

Access DB# 64892

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SHENGJUN WANG Examiner #: 77601 Date: 2-20-02
Art Unit: 1612 Phone Number 308-4554 Serial Number: 091523,776
Mail Box and Bldg/Room Location: 2E14 Results Format Preferred (circle): PAPER DISK E-MAIL

2B19
If more than one search is submitted, please prioritize searches in order of need. mej

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched.
Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Modulation of protein expression using carboxylic acyl alkanolic acid
Inventors (please provide full names): Pamela L. Zeitlin, Saul Brusilow

RECEIVED
MAR 22 2002
Earliest Priority Filing Date: 3/11/2000

For Sequence Searches Only: Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Search compounds defined in claims and ^{their} employment as therapeutic agent, and for treating cystic fibrosis!
See attached claims 1, 5, 15, 16 and 24

STAFF USE ONLY

Type of Search

Vendors and cost where applicable

Searcher Phone #: 308-4499

AA Sequence (#) _____

Dialog _____

Searcher Location: _____

Structure (#) _____

Questel/Orbit _____

Date Searcher Picked Up: _____

Bibliographic _____

Dr.Link _____

Date Completed: 5/8/02

Litigation _____

Lexis/Nexis _____

Searcher Prep & Review Time: _____

Fulltext _____

Sequence Systems _____

Clerical Prep Time: _____

Patent Family _____

WWW/Internet _____

Online Time: _____

Other _____

Other (specify) _____

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 14:29:01 ON 08 MAY 2002

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FILE COVERS 1907 - 8 May 2002 VOL 136 ISS 19

FILE LAST UPDATED: 6 May 2002 (20020506/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

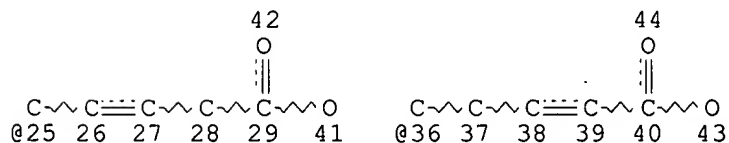
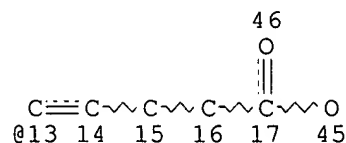
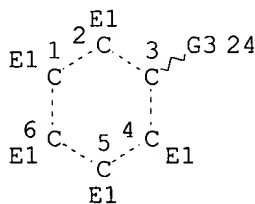
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L33 STR



VAR G3=13/25/36

NODE ATTRIBUTES:

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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

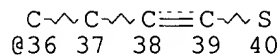
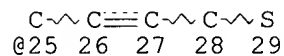
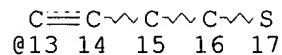
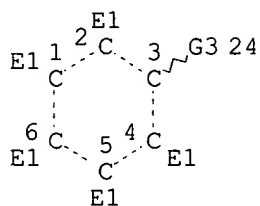
RSPEC I

NUMBER OF NODES IS 28

STEREO ATTRIBUTES: NONE

L35 4532 SEA FILE=REGISTRY SSS FUL L33

L36 STR



VAR G3=13/25/36

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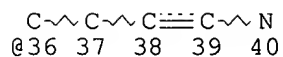
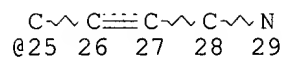
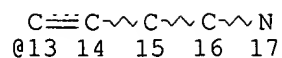
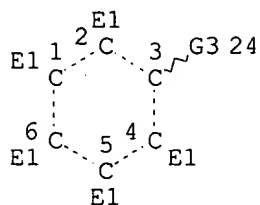
GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L38 STR



VAR G3=13/25/36

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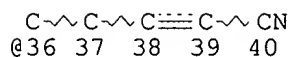
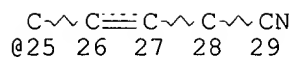
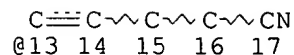
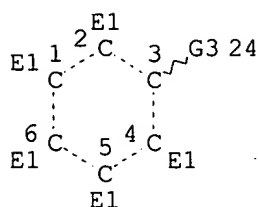
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RSPEC I

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L39 STR



VAR G3=13/25/36

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

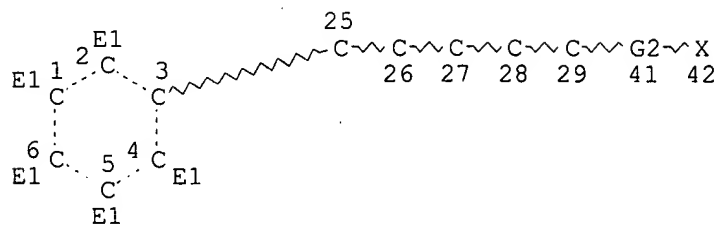
GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L46 STR



REP G2=(0-5) C

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HCOUNT	IS	E1	AT	6

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L49 11858 SEA FILE=REGISTRY SSS FUL L36 OR L38 OR L39 OR L46

L50 15572 SEA FILE=REGISTRY ABB=ON PLU=ON L35 OR L49

L51 8713 SEA FILE=HCAPLUS ABB=ON PLU=ON L50

L54 0 SEA FILE=HCAPLUS ABB=ON PLU=ON L51(L) (?CYSTIC(5A)FIBRO?)

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L33 STR
 L35 4532 SEA FILE=REGISTRY SSS FUL L33
 L36 STR
 L38 STR
 L39 STR
 L46 STR
 L49 11858 SEA FILE=REGISTRY SSS FUL L36 OR L38 OR L39 OR L46
 L50 15572 SEA FILE=REGISTRY ABB=ON PLU=ON L35 OR L49
 L51 8713 SEA FILE=HCAPLUS ABB=ON PLU=ON L50
 L58 47 SEA FILE=HCAPLUS ABB=ON PLU=ON L51(L) (LUNG OR (SURFACTANT OR
 TRANSMEMBRAN?) (5A) PROTEIN OR ?RESPIR? OR CF OR CFTR OR LIVER
 OR ?TRYPSIN? OR ?ALZHEIM? OR ?MARFAN? OR ?CHOLESTEROL? OR
 TAY(W)SACH?)

=>.d ibib abs hitrn 158 1-47

L58 ANSWER 1 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2002:251850 HCAPLUS
 DOCUMENT NUMBER: 136:273206
 TITLE: Combination therapy for treating hypercholesterolemia
 using a bile acid sequestrant polymer and a
 cholesterol-lowering agent
 INVENTOR(S): Huval, Chad Cori; Holmes-Farley, Stephen Randall;
 Petersen, John S.; Dhal, Pradeep K.
 PATENT ASSIGNEE(S): Geltex Pharmaceuticals, Inc., USA
 SOURCE: U.S., 12 pp., Cont.-in-part of U.S. 6,083,497.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6365186	B1	20020402	US 1999-311103	19990513
ZA 9809673	A	19990511	ZA 1998-9673	19981023
US 6248318	B1	20010619	US 2000-521975	20000309

PRIORITY APPLN. INFO.: US 1997-964536 A2 19971105

AB A method for treating hypercholesterolemia and atherosclerosis, and
 reducing serum cholesterol comprise administering to a mammal a compn.
 contg. a bile acid sequestrant compd. which is an unsubstituted
 polydiallylamine polymer and a cholesterol-lowering agent, and optionally
 a pharmaceutically acceptable carrier. Crosslinked polydiallylamine is a
 highly potent bile acid sequestrant, with in vivo activity greater than
 current com. products. For example, epichlorohydrin-crosslinked
 polydiallylamine was prepd. and when given to hamster at a daily dose of
 0.10-0.25% in feed it induced fecal excretion of bile acids of 2.19-3.48
 .mu.mol/g, compared to 1.34 .mu.mol/g fecal bile acids with no polymer in
 feed.

IT 7236-47-7, .beta.-Benzalbutyramide

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (combination of polydiallylamine polymer as bile acid sequestrant and
 cholesterol-lowering agent for treating
 hypercholesterolemia and atherosclerosis)

REFERENCE COUNT: 108 THERE ARE 108 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L58 ANSWER 2 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:824114 HCAPLUS
 DOCUMENT NUMBER: 134:530
 TITLE: Polydiallylamine bile acid sequestrant-
 hypocholesterolemic agent combination for treating
 hypercholesterolemia
 INVENTOR(S): Huval, Chad Cori; Holmes-Farley, Stephen Randall;
 Petersen, John S.; Dhal, Pradeep K.
 PATENT ASSIGNEE(S): Geltex Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000069445	A1	20001123	WO 1999-US10568	19990513
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 9939880	A1	20001205	AU 1999-39880	19990513

PRIORITY APPLN. INFO.: WO 1999-US10568 A 19990513

AB Methods are provide for treating hypercholesterolemia and atherosclerosis, and reducing serum cholesterol in a mammal. The methods of the invention comprise administering to a mammal a first amt. of a bile acid sequestrant compd. which is an unsubstituted polydiallylamine polymer and a second amt. of a cholesterol-lowering agent. The first and second amts. together comprise a therapeutically effective amt. The invention further provides pharmaceutical compns. useful for the treatment of hypercholesterolemia and atherosclerosis, and for reducing serum cholesterol. The pharmaceutical compns. comprise a combination of a first amt. of an unsubstituted polydiallylamine polymer compd. and a second amt. of a cholesterol-lowering agent. The first and second amts. comprise a therapeutically effective amt. The pharmaceutical compns. of the present invention may optionally contain a pharmaceutically acceptable carrier.

IT 7236-47-7, .beta.-Benzalbutyramide

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(polydiallylamine bile acid sequestrant-hypocholesterolemic agent combination for treating hypercholesterolemia)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 3 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:601227 HCAPLUS
 DOCUMENT NUMBER: 133:296331
 TITLE: Synthesis of 3-arylpropenyl, 3-arylpropynyl and
 3-arylpropyl 2-azetidinones as cholesterol absorption

inhibitors: application of the palladium-catalyzed arylation of alkenes and alkynes

AUTHOR(S): Rosenblum, Stuart B.; Huynh, Tram; Afonso, Adriano; Davis, Harry R., Jr.

CORPORATE SOURCE: Chemistry Department, Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Tetrahedron (2000), 56(31), 5735-5742
CODEN: TETRAB; ISSN: 0040-4020

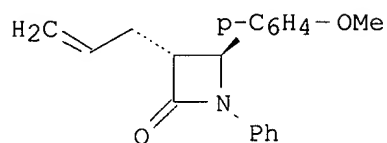
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:296331

GI



AB A series of N,2-diaryl-3-(3'-arylpropenyl)-2-azetidinones and N,2-diaryl-3-(3'-arylpropynyl)-2-azetidinones were prepd. by the palladium-catalyzed arylation of I or by arylation of 4-pentenoic acid, or via Et 4-pentynoate followed by 2-azetidinone ring construction. These unsatd. 2-azetidinones were transformed to their satd. analogs by catalytic hydrogenation. These unsatd. and satd. synthesized azetidinones were evaluated for their biol. activity as cholesterol absorption inhibitors in hamsters.

IT 300662-69-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 3-arylpropenyl-, 3-arylpropynyl- and 3-arylpropyl-2-azetidinones as **cholesterol** absorption inhibitors)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 4 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:768050 HCAPLUS

DOCUMENT NUMBER: 130:52236

TITLE: Preparation of dihydroxyphthalic acid diethers as squalene synthase inhibitors, their pharmaceutical uses, and their intermediates

INVENTOR(S): Ichikawa, Yuichiro; Niizuma, Setsuko; Abe, Masatoshi; Takahashi, Wataru; Ikeda, Tatsuji; Takashio, Kazutoshi

PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 64 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

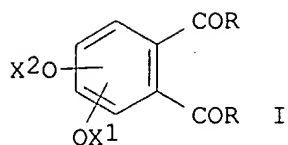
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10316617	A2	19981202	JP 1997-141169	19970516
OTHER SOURCE(S): MARPAT 130:52236				

GI



AB The title derivs. I [R = OH: X1, X2 = (un)substituted linear or branched C1-20 (un)satd. aliph. hydrocarbyl, (un)substituted C2-8 alkyloxyalkyl, alkenyloxyalkyl, YZ [Y = (un)substituted C1-8 (hydroxy)alkyl, (un)substituted C2-8 alkyloxyalkyl, (un)substituted C2-8 alkylaminoalkyl; Z = (un)substituted aryl] (II); except the case where X1 = X2 = C1-3 alkyl, benzyl] and/or their pharmaceutically acceptable salts are prepd. by hydrolyzing I [R = OR1, NR2R3; R1-3 = C1-6 alkyl, (un)substituted C7-10 aralkyl; X1, X2 = same as in II]. II and their salts are useful for treatment of infection, hypercholesterolemia, hyperlipemia, or atherosclerosis. IC50 of 3-farnesyloxy-4-[4-(3-phenoxyphenyl)butoxy]phthalic acid (prepn. given) against *Aspergillus fumigatus* squalene synthase was 0.41 .mu.g/mL. Antifungal activity against *A. fumigatus* and *Candida albicans*, and cholesterol formation-inhibiting action of II were also shown.

IT **52121-98-9**, 1-Iodo-6-phenylhexane **99858-37-4**, (5-Iodopentyl)benzene

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of dihydroxyphthalic acid diethers as squalene synthase inhibitors for treatment of fungal infection and hypercholesterolemia)

L58 ANSWER 5 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:660120 HCAPLUS

DOCUMENT NUMBER: 130:3720

TITLE: 2-azetidinone cholesterol absorption inhibitors: increased potency by substitution of the C-4 phenyl ring

AUTHOR(S): Vaccaro, Wayne D.; Sher, Rosy; Davis, Harry R., Jr.
CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ, 07033-0539, USA

SOURCE: Bioorganic & Medicinal Chemistry (1998), 6(9), 1429-1437

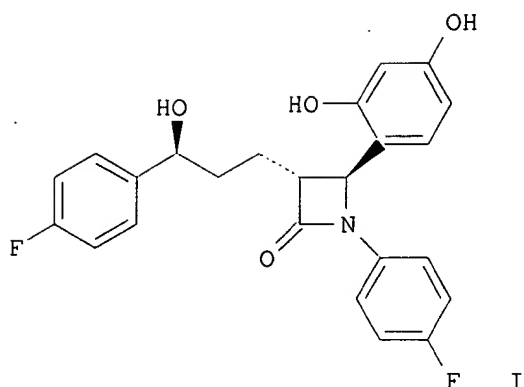
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB SAR studies directed towards the optimization of 2-azetidinone cholesterol absorption inhibitors led to the discovery of I, the most potent cholesterol absorption inhibitor yet identified.

IT 20371-41-9, 5-Phenylvaleryl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)
(effect of substitution of the C-4 Ph ring on 2-azetidinone
cholesterol absorption inhibitors)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 6 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:632344 HCAPLUS

DOCUMENT NUMBER: 129:330578

TITLE: Beta-lactams derived from the reaction of phenanthridiones and 11H-dibenzo[b,e]azepin-11-one with phenylvaleryl chloride. Synthesis of fused analogs of the cholesterol absorption inhibitor Sch 48461

AUTHOR(S): Afonso, Adriano; Rosenblum, Stuart B.; Puar, Mohindar S.; McPhail, Andrew T.

CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Tetrahedron Lett. (1998), 39(41), 7431-7434
CODEN: TELEAY; ISSN: 0040-4039

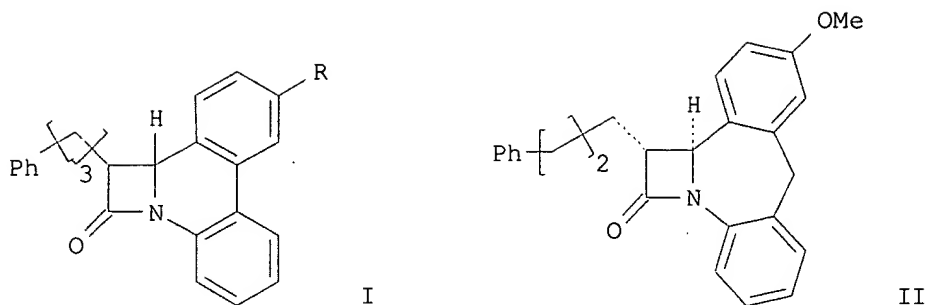
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:330578

GI



AB Phenanthridine and 9-methoxyphenanthridine and 11H-dibenzo[b,e]azepin-11-one were used as the imine components in the ketene-imine .beta.-lactam synthesis to provide the fused tetracyclic .beta.-lactams (I) (R = H, OMe) and (II).

IT 20371-41-9, 5-Phenylpentanoyl chloride

RL: RCT (Reactant)

(synthesis of fused analogs of the **cholesterol** absorption inhibitor Sch 48461)

L58 ANSWER 7 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:352625 HCAPLUS

DOCUMENT NUMBER: 129:41376

TITLE: Preparation of sugar-substituted 2-azetidinones useful as hypocholesterolemic agents

INVENTOR(S): Yumibe, Nathan P.; Alton, Kevin B.; Van Heek, Margaret; Davis, Harry R.; Vaccaro, Wayne D.

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: U.S., 18 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

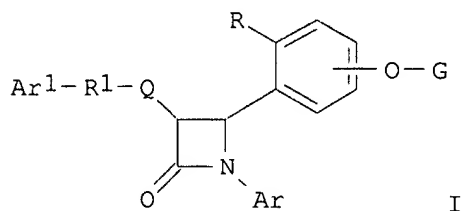
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5756470	A	19980526	US 1996-741179	19961029
CN 1205707	A	19990120	CN 1996-199226	19961029
PRIORITY APPLN. INFO.:			US 1996-741179	19961029
OTHER SOURCE(S):	MARPAT 129:41376			

GI



AB Hypocholesterolemic sugar-substituted 2-azetidinones I (R = H, OH, sugar; R1 = alkylene, cycloalkylene, phenylene, alkenylene; G = sugar residue; Q = bond, spiro group; Ar, Ar1 = aryl), are disclosed, as well as a method of lowering cholesterol by administering said compds., pharmaceutical compns. contg. them, and the combination of a sugar-substituted 2-azetidinone cholesterol-lowering agent and a cholesterol biosynthesis inhibitor for the treatment and prevention of atherosclerosis. Thus, 1-O-[4-[trans-(3R,4S)-1-(4-fluorophenyl)-2-oxo-3-[3-[(S)-hydroxy-4-fluorophenylpropyl]]-4-azetidiny]]phenyl]-.beta.-D-glucuronic acid was prepd. as anticholesteremic agent 58 % redn. in plasma cholesterol with 3 mg/kg dose in hamsters.

IT 20371-41-9, 5-Phenylvaleryl chloride
 RL: RCT (Reactant)
 (prepn. of sugar substituted azetidinones useful as
 hypocholesterolemic agents)

L58 ANSWER 8 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:168443 HCAPLUS

DOCUMENT NUMBER: 128:291977

TITLE: A novel type of structurally simple nonpeptide inhibitors for .alpha.-chymotrypsin. Induced-fit binding of methyl 2-allyl-3-benzenepropanoate to the S2 subsite pocket

AUTHOR(S): Kim, Dong H.; Li, Zhi-Hong; Lee, Soo Suk; Park, Jeong-Il; Chung, Sang J.

CORPORATE SOURCE: Center for Biofunctional Molecules and Department of Chemistry, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Bioorg. Med. Chem. (1998), 6(2), 239-249

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Unexpectedly, Me and benzyl esters of 2-allyl-3-benzenepropanoic acid were found to be not substrates but potent competitive inhibitors for .alpha.-chymotrypsin. The inhibitory property of the structurally simple nonpeptidic compds. is ascribed to their high binding affinity to the enzyme at the S2 rather than S1 subsite pocket. These inhibitors exist in a flexible form in soln., but as they bind to the enzyme bulky constrained conformers present in a minute concn. play an important role, forming tighter enzyme inhibitor complexes by binding to the large hydrophobic S2 pocket. The constrained conformers are thought to result from intramol. CH/.pi. interactions between a vinylic proton and the arom. .pi.-electron cloud in the inhibitor mols.

IT 205373-53-1P

RL: BYP (Byproduct); PREP (Preparation)
 (inhibition of .alpha.-**chymotrypsin** by
 allylbenzenepropanoates)

IT 205373-47-3P 205373-49-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (inhibition of .alpha.-**chymotrypsin** by
 allylbenzenepropanoates)

L58 ANSWER 9 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:119628 HCAPLUS

DOCUMENT NUMBER: 128:225681

TITLE: Discovery of 1-(4-Fluorophenyl)-(3R)-[3-(4-fluorophenyl)-(3S)-hydroxypropyl]-(4S)-(4-hydroxyphenyl)-2-azetidinone (SCH 58235): A Designed,

Potent, Orally Active Inhibitor of Cholesterol Absorption

AUTHOR(S): Rosenblum, Stuart B.; Huynh, Tram; Afonso, Adriano; Davis, Harry R., Jr.; Yumibe, Nathan; Clader, John W.; Burnett, Duane A.

CORPORATE SOURCE: Department of Discovery Research, Schering-Plough Research Institute, Kenilworth, NJ, 07033-0539, USA

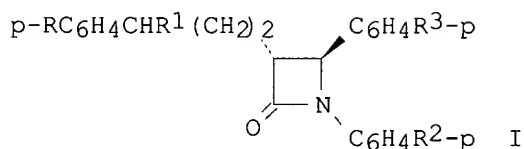
SOURCE: J. Med. Chem. (1998), 41(6), 973-980
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB (3R)-(3-Phenylpropyl)-1, (4S)-bis(4-methoxyphenyl)-2-azetidinone, SCH 48461 (I, R = R¹ = H, R² = R³ = OMe), a novel inhibitor of intestinal cholesterol absorption, was recently described by Burnett et al. and demonstrated to lower total plasma cholesterol in man. The potential sites of metab. of SCH 48461 were considered, and the most probable metabolites were prepd. The oral cholesterol-lowering efficacy of the putative metabolites was evaluated in a 7-day cholesterol-fed hamster model for the redn. of serum total cholesterol and liver cholesteryl esters vs. control. The putative metabolite structure-activity relationship (SAR) of 1-(4-fluorophenyl)-(3R)-[3-(4-fluorophenyl)-(3S)-hydroxypropyl]-(4S)-(4-hydroxyphenyl)-2-azetidinone, SCH 58235 (I, R = R² = F, R¹ = .beta.-OH, R³ = OH), was designed to exploit activity enhancing oxidn. and to block sites of potential detrimental metabolic oxidn. A series of congeners of SCH 48461 were prepd. incorporating strategically placed hydroxyl groups and fluorine atoms to further probe the SAR of 2-azetidinone cholesterol absorption inhibitors. Through the SAR anal. of a series of putative metabolites of SCH 48461, compd. SCH 58235 was targeted and found to exhibit remarkable efficacy with an ED₅₀ of 0.04 mg/kg/day for the redn. of liver cholesteryl esters in a 7-day cholesterol-fed hamster model.

IT 20371-41-9, Benzenepentanoyl chloride
 RL: RCT (Reactant)
 (prepn. of 1-(4-fluorophenyl)-(3R)-[3-(4-fluorophenyl)-(3S)-hydroxypropyl]-(4S)-(4-hydroxyphenyl)-2-azetidinone (SCH 58235) designed as an inhibitor of **cholesterol** absorption)

L58 ANSWER 10 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:761872 HCAPLUS

DOCUMENT NUMBER: 128:30416

TITLE: Use of nonpeptide bradykinin antagonists for treating and preventing chronic fibrogenetic liver diseases, acute liver diseases and complications thereof

INVENTOR(S): Heitsch, Holger; Wagner, Adalbert; Wirth, Klaus; Hropot, Max; Bickel, Martin

PATENT ASSIGNEE(S): Hoechst A.-G., Germany
 SOURCE: Eur. Pat. Appl., 36 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 808628	A2	19971126	EP 1997-108096	19970520
EP 808628	A3	19980114		
EP 808628	B1	20000202		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI				
DE 19620509	A1	19971127	DE 1996-19620509	19960522
DE 19632042	A1	19980212	DE 1996-19632042	19960808
DE 19639303	A1	19980326	DE 1996-19639303	19960925
US 5786365	A	19980728	US 1997-858550	19970519
AU 9723511	A1	19971127	AU 1997-23511	19970520
AT 189389	E	20000215	AT 1997-108096	19970520
ES 2144291	T3	20000601	ES 1997-108096	19970520
NO 9702311	A	19971124	NO 1997-2311	19970521
ZA 9704415	A	19971124	ZA 1997-4415	19970521
JP 10045624	A2	19980217	JP 1997-131160	19970521
CN 1176102	A	19980318	CN 1997-113108	19970521
CA 2205780	AA	19971122	CA 1997-2205780	19970522
BR 9703367	A	19980915	BR 1997-3367	19970522

PRIORITY APPLN. INFO.:

DE 1996-19620509 A 19960522
 DE 1996-19632042 A 19960808
 DE 1996-19639303 A 19960925

AB Forty-five heterocyclic compds. are pictured which act as bradykinin antagonists and which can be used in the title syndromes (e.g., liver cirrhosis and liver fibrosis).

IT 199791-52-1

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (liver diseases treatment by)

L58 ANSWER 11 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:761871 HCAPLUS

DOCUMENT NUMBER: 128:30415

TITLE: Use of nonpeptide bradykinin antagonists for treating and preventing chronic fibrogenetic liver diseases, acute liver diseases and complications thereof

INVENTOR(S): Heitsch, Holger; Wagner, Adalbert; Wirth, Klaus; Hropot, Max; Bickel, Martin

PATENT ASSIGNEE(S): Hoechst A.-G., Germany
 SOURCE: Eur. Pat. Appl., 32 pp.
 CODEN: EPXXDW

DOCUMENT TYPE: Patent
 LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 808627	A2	19971126	EP 1997-107624	19970509
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,				

SI, FI

DE 19620509	A1	19971127	DE 1996-19620509	19960522
DE 19632042	A1	19980212	DE 1996-19632042	19960808
DE 19639303	A1	19980326	DE 1996-19639303	19960925
US 5786365	A	19980728	US 1997-858550	19970519
AU 9723511	A1	19971127	AU 1997-23511	19970520
AT 189389	E	20000215	AT 1997-108096	19970520
ES 2144291	T3	20000601	ES 1997-108096	19970520
NO 9702311	A	19971124	NO 1997-2311	19970521
ZA 9704415	A	19971124	ZA 1997-4415	19970521
JP 10045624	A2	19980217	JP 1997-131160	19970521
CN 1176102	A	19980318	CN 1997-113108	19970521
CA 2205780	AA	19971122	CA 1997-2205780	19970522
BR 9703367	A	19980915	BR 1997-3367	19970522

PRIORITY APPLN. INFO.:

DE 1996-19620509 A 19960522
 DE 1996-19632042 A 19960808
 DE 1996-19639303 A 19960925

AB Forty-five heterocyclic compds. are pictured which act as bradykinin antagonists and which can be used in the title syndromes (e.g., liver cirrhosis and liver fibrosis).

IT 199791-52-1

RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (liver diseases treatment by)

L58 ANSWER 12 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:752738 HCAPLUS

DOCUMENT NUMBER: 128:34672

TITLE: Substituted azetidinone compounds useful as hypocholesterolemic agents

INVENTOR(S): Vaccaro, Wayne D.

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: U.S., 12 pp. Cont.-in-part of U.S. Ser. No. 261,785, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

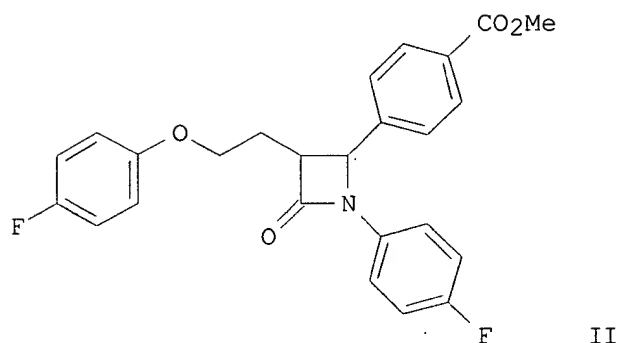
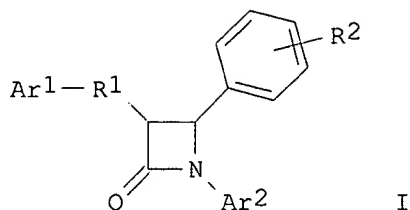
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5688785	A	19971118	US 1995-449973	19950525
AU 9223980	A1	19930223	AU 1992-23980	19920721
AU 658441	B2	19950413		
ZA 9205487	A	19930331	ZA 1992-5487	19920721
EP 596015	A1	19940511	EP 1992-916790	19920721
EP 596015	B1	19971001		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06508637	T2	19940929	JP 1992-502964	19920721
JP 2525125	B2	19960814		
LV 10429	B	19950820	LV 1992-550	19921229
LT 3369	B	19950825	LT 1992-261	19921229
NO 9400221	A	19940121	NO 1994-221	19940121
US 5688787	A	19971118	US 1996-588785	19960119

PRIORITY APPLN. INFO.:

US 1991-734426 B2 19910723
 US 1991-734652 B2 19910723
 US 1994-178312 B2 19940111
 US 1994-261785 B2 19940620

OTHER SOURCE(S): MARPAT 128:34672
GI



AB Substituted azetidinone hypocholesterolemic agents I and their pharmaceutically acceptable salts are disclosed [wherein: Ar1 = aryl or R3-substituted aryl; Ar2 = aryl or R4-substituted aryl; R1 = (CH2)2-6, (CH2)eZ(CH2)r (wherein Z = O, CO, C6H4, NR10, or S(O)0-2, e = 0-5, and r = 0-5, provided that (e + r) = 1-6), C2-6 alkenylene, and (CH2)fV(CH2)g (wherein V = C3-6 cycloalkylene, f = 1-5, and g = 0-5, provided that (f + g) = 1-6); R2 = alkylene-COR5 or CH:CHCOR5; R3, R4 = 1-3 substituents chosen from alkyl, OR6, OCOR6, OCOOR9, O(CH2)1-5OR6, OCONR6R7, NR6R7, NR6COR7, NR6CO2R9, NR6CONR7R8, NR6SO2R9, COOR6, CONR6R7, COR6, SO2NR6R7, S(O)0-2R9, O(CH2)1-10COOR6, O(CH2)1-10CONR6R7, alkylene-COOR6, CH:CHCO2R6, CF3, CN, NO2, and halo; R5 = OR or NRR12 (wherein R and R12 = H, alkyl, aryl, and aralkyl); R6, R7, R8 = H, lower alkyl, aryl, and aralkyl; R9 = alkyl, aryl, or aralkyl; R10 = H, alkyl, aralkyl, or COR6]. I are cholesterol absorption inhibitors, which may be used (no data) in combination with cholesterol biosynthesis inhibitors. For example, Me 4-formylbenzoate was condensed with 4-FC6H4NH2 in PhMe under Dean-Stark conditions, and the resulting imine was cyclized in situ with 4-FC6H4O(CH2)3COCl in the presence of Bu3N at reflux to give an 8:1 trans/cis mixt. of azetidinone II. The mixt. was sepd. into the pure isomers by HPLC. At 50 mg/kg orally in hamsters, trans-II gave 28% redn. of serum cholesterol, and 76% redn. of cholesterol esters.

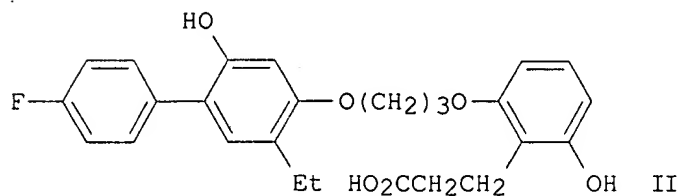
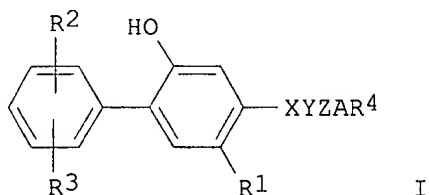
IT 20371-41-9, 5-Phenylvaleryl chloride

RL: RCT (Reactant)

(prepn. of substituted azetidinones as hypocholesterolemic agents)

L58 ANSWER 13 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:53684 HCAPLUS
 DOCUMENT NUMBER: 126:74591
 TITLE: Preparation of biphenylyloxyalkylarenes as leukotriene antagonists for the treatment or prevention of Alzheimer's disease.
 INVENTOR(S): Altstiel, Larry Douglas; Fleisch, Jerome Herbert
 PATENT ASSIGNEE(S): Lilly, Eli, and Co., USA
 SOURCE: Eur. Pat. Appl., 124 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 743064	A1	19961120	EP 1996-303346	19960513
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
WO 9636347	A1	19961121	WO 1996-US6773	19960513
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM				
RW: KE, LS, MW, SD, SZ, UG, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9658572	A1	19961129	AU 1996-58572	19960513
PRIORITY APPLN. INFO.:			US 1995-443179	19950517
			WO 1996-US6773	19960513
OTHER SOURCE(S):		MARPAT 126:74591		
GI				



AB Use of compds. having leukotriene antagonist activity, e.g., title compds. [I; R1 = alkyl, alkenyl, alkynyl, alkoxy, alkylthio, halo, R2-substituted Ph; R2, R3 = H, halo, OH, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, CF3, dialkylamino; X = O, S, CO, CH2; Y = O, CH2; XY =

CH:CH, C.tplbond.C; Z = alkylene; A = bond, O, S, CH:CH, etc.; R4 = (substituted) (hetero)aryl; with provisos] for manuf. of a medicament for treating or preventing Alzheimer's disease is claimed. Thus, 5-hydroxybenzopyran-2-one and 3-(2-ethyl-4-(4-fluorophenyl)-5-benzyloxyphenyl)propyl iodide were stirred with NaH in Me₂SO to give 5-[3-(2-ethyl-4-(4-fluorophenyl)-5-benzyloxyphenyl)propoxy]benzopyran-2-one. This was converted to title compd. (II), which displaced [3H]-LTB₄ from guinea pig lung membrane preps. with pK_i = 9.01. I drug formulations are given.

IT **14377-66-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of biphenyloxyalkylarenes as leukotriene antagonists for the treatment or prevention of **Alzheimer's** disease)

L58 ANSWER 14 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:513507 HCAPLUS

DOCUMENT NUMBER: 125:131668

TITLE: 2-Azetidinone Cholesterol Absorption Inhibitors:
Structure-Activity Relationships on the Heterocyclic
Nucleus

AUTHOR(S): Clader, John W.; Burnett, Duane A.; Caplen, Mary Ann;
Domalski, Martin S.; Dugar, Sundee; Vaccaro, Wayne;
Sher, Rosy; Browne, Margaret E.; Zhao, Hongrong; et
al.

CORPORATE SOURCE: Schering-Plough Research Institute, Kenilworth, NJ,
07033-0539, USA

SOURCE: J. Med. Chem. (1996), 39(19), 3684-3693

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of azetidinone cholesterol absorption inhibitors related to SCH 48461 was prepd., and evaluated for their ability to inhibit hepatic cholesteryl ester formation in a cholesterol-fed hamster model. Although originally designed as acyl CoA:cholesterol acyltransferase (ACAT) inhibitors, comparison of in vivo potency with in vitro activity in a microsomal ACAT assay indicates no correlation between activity in these 2 models. The mol. mechanism by which these compds. inhibit cholesterol absorption is unknown. Despite this limitation, examn. of the in vivo activity of a range of compds. has revealed clear structure-activity relationships consistent with a well-defined mol. target. The details of these structure-activity relationships and their implications on the nature of the putative pharmacophore are discussed.

IT **20371-41-9**, 5-Phenylpentanoyl chloride

RL: RCT (Reactant)

(structure-activity relations of azetidinone **cholesterol**
absorption inhibitors)

L58 ANSWER 15 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:479041 HCAPLUS

DOCUMENT NUMBER: 125:167712

TITLE: A simple stereoselective synthesis of the cholesterol
absorption inhibitor (-)-SCH 48461

AUTHOR(S): Braun, Manfred; Galle, Dietmar

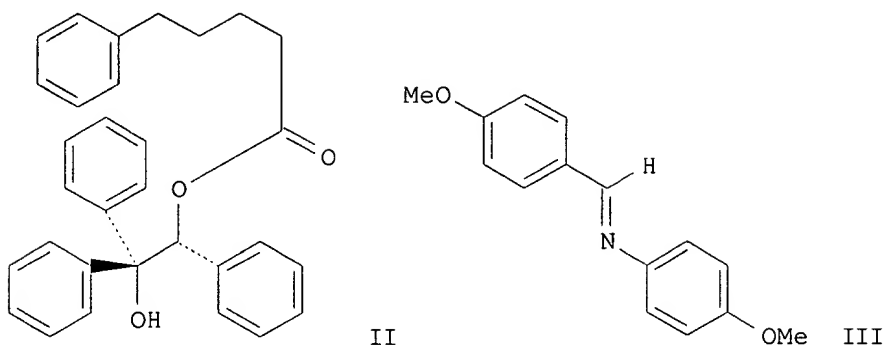
CORPORATE SOURCE: Institut Organische Chemie Makromolekulare Chemie,
Universitaet Duesseldorf, Duesseldorf, D-40225,
Germany

SOURCE: Synthesis (1996), (7), 819-820

CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English
 OTHER SOURCE(S): CASREACT 125:167712
 GI



AB The cholesterol absorption inhibitor I is synthesized in 91% ee by a stereoselective condensation of doubly deprotonated ester II and imine III. The optical purity of the trans-diastereomer obtained as the major isomer (trans/cis, 94:6) is enhanced to > 98% ee by a single recrystn.
 IT **20371-41-9**, Benzenepentanoyl chloride
 RL: RCT (Reactant)
 (prepn. of **cholesterol** absorption inhibitor (-)-SCH 48461)

L58 ANSWER 16 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:441078 HCAPLUS

DOCUMENT NUMBER: 125:184776

TITLE: In vitro metabolism of a potent HIV-protease inhibitor (141W94) using rat, monkey and human liver S9

AUTHOR(S): Singh, Rominder; Chang, Sai Y.; Taylor, Lester C. E.

CORPORATE SOURCE: Bioanalysis and Drug Metabolism, Glaxo Wellcome Inc., Research Triangle Park, NC, 27709, USA

SOURCE: Rapid Commun. Mass Spectrom. (1996), 10(9), 1019-1026
 CODEN: RCMSEF; ISSN: 0951-4198

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Compd. 141W94 (Vertex VX478) (3S)-tetrahydro-3-furyl N-[(S,2R)-3-(4-amino-N-isobutylbenzenesulfonamido)-1-benzyl-2-hydroxypropyl] carbamate, is a potent HIV-protease inhibitor and is currently undergoing clin. trials. The purpose of this study was the rapid identification of the phase I and II in vitro metabolite of 141W94 using mass spectrometry. Four different sources of liver S9 fractions were used for studying comparative in vitro metab. of 141W94. They were obtained from Arochlor-induced rat, normal (untreated) rat, cynomolgus monkey and human livers. Selected incubations were supplemented with uridine diphosphate glucuronic acid and the reduced form of glutathione. The predominant species seen in the incubation mixt. was the parent compd. 141W94. Metabolites arising from ring opening to form the diol and carboxylic acid and oxidn. of the THF ring (formation of dihydrofuran) were identified. In addn., of the two monohydroxylated products identified, one resulted from hydroxylation on the aniline ring and the other from hydroxylation at the benzylic position. Two different glucuronides were also obsd. Comparing the three species, very little metab. was seen in the normal (non-induced) rat. The metabolic profile

and extent of metab. with induced rat, monkey and human S9 was similar. Induced rat S9 incubation showed the formation of two unique metabolites that were not seen in non-induced rat, monkey and human S9 fractions. They were the monohydroxylated glucuronide and a carbamate cleavage product. The metabolites were identified using mass spectrometry based on their mol. masses and fragmentation patterns.

IT 180728-05-6

RL: MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(In vitro metab. of a potent HIV-protease inhibitor (141W94) using rat, monkey and human **liver** S9)

L58 ANSWER 17 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:425252 HCAPLUS

DOCUMENT NUMBER: 125:86319

TITLE: Preparation and formulation of N-(4-phenylcyclohexyl)alkanamides and analogs as cholesterol biosynthesis inhibitors

INVENTOR(S): Maier, Roland; Mueller, Peter; Woitun, Eberhard;
Hurnaus, Rudolf; Mark, Michael; Eisele, Bernhard;
Budzinski, Ralph-Michael

PATENT ASSIGNEE(S): Dr. Karl Thomae GmbH, Germany

SOURCE: Ger. Offen., 40 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

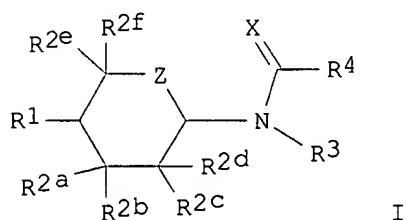
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4437999	A1	19960502	DE 1994-4437999	19941025

OTHER SOURCE(S) : MARPAT 125:86319

GI



I

AB Title compds. [I; R1 = substituted Ph, pyridyl, pyrimidinyl, etc.; Z = (CR2hR2g)n; R2a-R2h = H, alk(en)yl; R3 = alk(en)yl, alkynyl, Ph, cyclohexyl(methyl); R4 = (O- or S-interrupted) alkyl, alkenyl, phenyl(alkyl), etc.; X = O, S, NPh, NSO2C6H4Me-4; n = 0 or 1] were prepd. Thus, I, e.g., prepd. 4-[4-(2-diethylaminoethoxy)-3-methylphenyl]-N-hexanoyl-N-methylcyclohexylamine gave .gtoreq.50% inhibition of cholesterol biosynthesis in human hepatoma cells at 10-6M in vitro.

IT 178540-24-4P 178540-37-9P 178540-64-2P

178541-15-6P 178541-89-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and formulation of N-(4-phenylcyclohexyl)alkanamides and analogs as **cholesterol** biosynthesis inhibitors)

L58 ANSWER 18 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:404621 HCAPLUS

DOCUMENT NUMBER: 125:58115

TITLE: Preparation of N-benzyl-N-acylcycloalkylamine-derivative cholesterol biosynthesis inhibitors

INVENTOR(S): Maier, Roland; Woitun, Eberhard; Mueller, Peter; Hurnaus, Rudolf; Mark, Michael; Eisele, Bernhard; Budzinski, Ralph-Michael

PATENT ASSIGNEE(S): Dr. Karl Thomae GmbH, Germany

SOURCE: Ger. Offen., 31 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

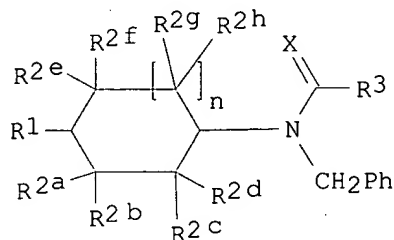
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4438055	A1	19960502	DE 1994-4438055	19941025

OTHER SOURCE(S): MARPAT 125:58115
GI



I

AB The title compds. [I; R1 = (un)branched alkyl, PhCH2, (un)substituted Ph, naphthyl, heterocyclyl, etc.; R2a-R2h = H, alkyl, allyl; R3 = H, (un)branched (un)substituted alkyl, (un)substituted alkenyl, etc.; X = O, S, (un)substituted NH; n = 0-1], useful as cholesterol biosynthesis inhibitors (no data) via the inhibition of HMG-CoA reductase (no data), useful for the treatment of hyperlipidemia (no data) and atherosclerosis (no data), are prepd. and I-contg. formulations presented. Thus, trans-N-benzyl-4-(4-methoxy-3-methylphenyl)cyclohexylamine was amidated with hexanoyl chloride, producing trans-N-benzyl-N-hexanoyl-4-(4-methoxy-3-methylphenyl)cyclohexylamine in 96.3% theor. yield.

IT 178365-08-7P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-benzyl-N-acylcycloalkylamine-deriv. **cholesterol** biosynthesis inhibitors)

L58 ANSWER 19 OF 47 HCAPLUS COPYRIGHT 2002 ACS

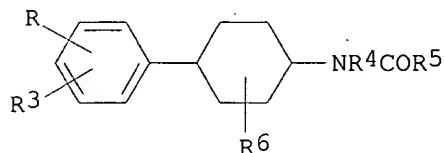
ACCESSION NUMBER: 1996:388195 HCAPLUS

DOCUMENT NUMBER: 125:58083

TITLE: Preparation of N-acylphenylcyclohexylamines as cholesterol biosynthesis inhibitors
 INVENTOR(S): Maier, Roland; Woitun, Eberhard; Mueller, Peter; Hurnaus, Rudolf; Mark, Michael; Eisele, Bernhard; Budzinski, Ralph-Michael
 PATENT ASSIGNEE(S): Dr. Karl Thomae GmbH, Germany
 SOURCE: Ger. Offen., 24 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4438020	A1	19960502	DE 1994-4438020	19941025

OTHER SOURCE(S): MARPAT 125:58083
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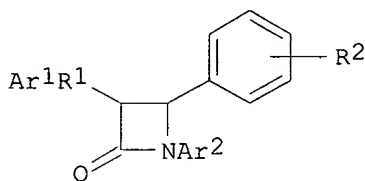
AB Title compds. [I; R = (CH₂)_nNR₁R₂; R₁, R₂ = H, alkyl, acyl; NR₁R₂ = pyrrolidino, piperidino, morpholino; R₃, R₆ = H or alkyl; R₄ = (cyclo)alkyl, allyl; Ph, etc.; R₅ = (phenyl)alk(en)yl, cycloalkyl, Ph, naphthyl, etc.; n = 0-3]. Thus, trans-N-acetyl-N-benzyl-4-(4-diethylaminomethylphenyl)cyclohexylamine, e.g., gave >50% inhibition of cholesterol biosynthesis in human hepatoma cells in vitro.

IT **178162-88-4P 178163-33-2P**
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of N-acylphenylcyclohexylamines as **cholesterol** biosynthesis inhibitors)

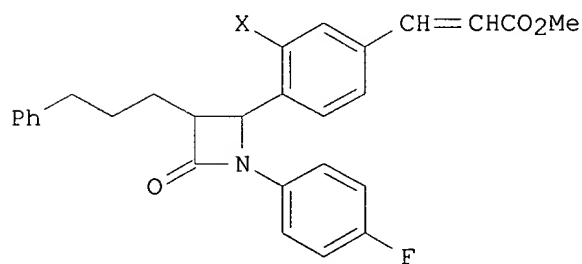
L58 ANSWER 20 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:214748 HCAPLUS
 DOCUMENT NUMBER: 124:316969
 TITLE: Substituted azetidinone compounds useful as hypocholesterolemic agents
 INVENTOR(S): Vaccaro, Wayne
 PATENT ASSIGNEE(S): Schering Corp., USA
 SOURCE: PCT Int. Appl., 31 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 5
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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 WO 9535277 A1 19951228 WO 1995-US7117 19950615
 W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG,
 KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG,
 SI, SK, TJ, TM, TT, UA, UZ, VN
 RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
 LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
 SN, TD, TG
 CA 2191455 AA 19951228 CA 1995-2191455 19950615
 AU 9529430 A1 19960115 AU 1995-29430 19950615
 EP 766667 A1 19970409 EP 1995-925237 19950615
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
 JP 10501811 T2 19980217 JP 1995-502289 19950615
 PRIORITY APPLN. INFO.: US 1994-261785 A 19940620
 WO 1995-US7117 W 19950615
 OTHER SOURCE(S): MARPAT 124:316969
 GI



I



II

AB Substituted azetidinone hypocholesterolemic agents are disclosed, specifically I and their pharmaceutically acceptable salts [wherein Ar1, Ar2 = (un)substituted aryl; R1 = (CH2)q, (CH2)eZ(CH2)r, C2-6 alkenylene, (CH2)fV(CH2)g; q = 2-6; Z = O, CO, C6H4, NR10, S(O)0-2; e, r = 0-5, provided that (e + r) = 1-6; V = C3-6 cycloalkylene; f = 1-5; g = 0-5, provided that (f + g) = 1-6; R2 = (lower alkylene)COR5 or (CH:CH)COR5; R5 = OR or NRR12; R, R12 = H, alkyl, aryl, aralkyl; R10 = H, alkyl, aralkyl or acyl]. Also disclosed are a method of lowering serum cholesterol by administering I or salts, alone or in combination with a cholesterol biosynthesis inhibitor, and pharmaceutical compns. contg. I. Examples include 16 syntheses, 2 formulations, and a bioassay. For instance, Pd(PPh3)4-catalyzed coupling of trans-1-(4-fluorophenyl)-3-(3-phenylpropyl)-4-(4-bromo-2-benzyloxyphenyl)-2-azetidinone with Me acrylate in the presence of Et3N at 80.degree. gave 48% title compd. trans-II (X = PhCH2O). The similarly prepd. compd. trans-II (X = H), at a dose of 10 mg/kg orally in hyperlipidemic hamsters, gave a 21% redn. in serum cholesterol, and a 48% redn. in cholesterol esters.

IT 20371-41-9, 5-Phenylvaleryl chloride

RL: RCT (Reactant)
(starting material; prepn. of azetidinone derivs. as
hypocholesteroleemics)

L58 ANSWER 21 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:110119 HCAPLUS

DOCUMENT NUMBER: 124:169116

TITLE: Irreversible inhibitions of serine proteases by
peptidyl allylic halide derivatives

AUTHOR(S): Ohba, Tsuyoshi; Ikeda, Eitatsu; Wakayama, Jun; Takei,
Hisashi

CORPORATE SOURCE: Interdisciplinary Grad. Sch. Sci. Eng., Tokyo Inst.
Technol., Yokohama, 226, Japan

SOURCE: Bioorg. Med. Chem. Lett. (1996), 6(3), 219-24

CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Peptidyl 4-amino-5-phenyl-2-pentenyl bromide and chloride derivs. were
active-site directed irreversible inhibitors of .alpha.-chymotrypsin but
did not show any irreversible inhibitory activity toward porcine
pancreatic elastase.

IT 173866-63-2P 173866-64-3P 173866-67-6P

173866-68-7P 173866-69-8P 173866-70-1P

173866-71-2P 173866-72-3P 173866-73-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
preparation); BIOL (Biological study); PREP (Preparation)

(irreversible inhibition of .alpha.-**chymotrypsin** by
phenylalanine-based peptidyl allylic halides)

IT 116246-06-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(irreversible inhibition of .alpha.-**chymotrypsin** by
phenylalanine-based peptidyl allylic halides)

L58 ANSWER 22 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:403385 HCAPLUS

DOCUMENT NUMBER: 122:151403

TITLE: Treatment of amyloidosis associated with Alzheimer
disease using modulators of protein phosphorylation
Buxbaum, Joseph D.; Gandy, Samuel E.; Greengard, Paul

PATENT ASSIGNEE(S): The Rockefeller University, USA

SOURCE: U.S., 29 pp. Cont.-in-part of U.S. 5,242,932.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5385915	A	19950131	US 1993-73112	19930607
US 5242932	A	19930907	US 1991-809174	19911217
US 5538983	A	19960723	US 1994-236411	19940429
PRIORITY APPLN. INFO.:			US 1990-524202	19900516
			US 1991-809174	19911217
			US 1993-73112	19930607

AB A method is disclosed for regulating phosphorylation of proteins involved
in controlling processing or function of key proteins found in
intracellular neurofibrillary tangles and extracellular amyloid plaques
assocd. with Alzheimer disease, comprising introducing an effective amt.

of a kinase modulator or phosphatase modulator, the modulator capable of increasing or decreasing the rate of proteolytic processing, or modulating the function, of said key proteins. A cell/tissue culture method for screening agents modulating amyloid formation is also disclosed. The effects of e.g. okadaic acid on the prodn. of APPS, the secreted form of amyloid precursor protein, were opposite to those obsd. for .beta./A4 peptide. The reciprocal effects of increased protein phosphorylation on APPS prodn. and .beta./A4 peptide prodn. are consistent with the idea that APPs and .beta./A4 peptide may be derived from 2 competing pathways of APP metab.

IT 34807-41-5, Mezerein

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(protein phosphorylation modulators for **Alzheimer**
disease-assocd. amyloidosis treatment)

L58 ANSWER 23 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:517027 HCAPLUS

DOCUMENT NUMBER: 119:117027

TITLE: Substituted beta-lactam compounds useful as
hypcholesterolemic agents and processes for their
preparation

INVENTOR(S): Burnett, Duane A.; Clader, John W.; Thiruvengadam,
Tiruvettipuram K.; Tann, Chou Hong; Lee, Junning;
McAllister, Timothy; Colon, Cesar; Barton, Derek H.
R.; Breslow, Ronald; et al.

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: Eur. Pat. Appl., 98 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

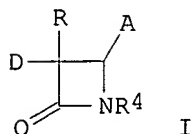
FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 524595	A1	19930127	EP 1992-112425	19920721
R: PT				
CA 2114007	AA	19930204	CA 1992-2114007	19920721
WO 9302048	A1	19930204	WO 1992-US5972	19920721
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO,				
PL, RO, RU, SD, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE, BF, BJ,				
CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9223980	A1	19930223	AU 1992-23980	19920721
AU 658441	B2	19950413		
ZA 9205487	A	19930331	ZA 1992-5487	19920721
EP 596015	A1	19940511	EP 1992-916790	19920721
EP 596015	B1	19971001		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06508637	T2	19940929	JP 1992-502964	19920721
JP 2525125	B2	19960814		
HU 67341	A2	19950328	HU 1994-185	19920721
AT 158789	E	19971015	AT 1992-916790	19920721
ES 2107548	T3	19971201	ES 1992-916790	19920721
CN 1069024	A	19930217	CN 1992-108760	19920722
LV 10429	B	19950820	LV 1992-550	19921229
LT 3369	B	19950825	LT 1992-261	19921229
NO 9400221	A	19940121	NO 1994-221	19940121
PRIORITY APPLN. INFO.:			US 1991-734426	A 19910723

US 1991-734652 A 19910723
 WO 1992-US5972 A 19920721

OTHER SOURCE(S): MARPAT 119:117027
 GI



AB Title compds. I (A = BCH:CH, BC.tplbond.C, BX(CH₂)_p wherein B = (substituted) Ph; X = bond, NH, S(O)_p, (substituted) heteroaryl, (substituted) benzofused heteroaryl, (substituted) piperazinyl(alkyl), etc., p = 0-2; R = H, F, C1-15 alkyl, C1-15 alkenyl, C1-15 alkynyl, B(CH₂)_h wherein h = 0-3, etc.; D = B'(CH₂)_mCO, B'(CH₂)_q, B'(C2-6 alkenylene, etc. wherein B' = naphthyl, (substituted) Ph, m = 1-5, q = 2-6; R₄ = substituted Ph, heterocyclyl) or a salt thereof, are prepd. (Me₂CH)₂NLi was added to Et 5-phenylvalerate in THF, followed by 4-methoxybenzylideneanisdine in CH₂Cl₂ to give the title (.+-.)-I (A = R₄ = 4-(MeO)C₆H₄, R = H, D = PhCH₂CH₂CH₂) (II). In hyperlipidemic hamsters, II at 50 mg/kg showed a redn. of serum cholesterol and cholesterol esters of 45 and 95%, resp. Capsule and tablet formulations comprising I are given.

IT 20371-41-9, Benzenepentanoyl chloride
 RL: RCT (Reactant)
 (reaction of, in prepn. of .beta.-lactam **hypocholesteroleemics**)

L58 ANSWER 24 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:446258 HCAPLUS

DOCUMENT NUMBER: 119:46258

TITLE: Protein kinase C-mediated pulmonary vasoconstriction in rabbit: Role of calcium, AA metabolites, and vasodilators

AUTHOR(S): Michael, John R.; Yang, Jianing; Farrukh, Imad S.; Gurtner, Gail H.

CORPORATE SOURCE: Med. Serv., Veterans Aff. Med. Cent., Salt Lake City, UT, 84132, USA

SOURCE: J. Appl. Physiol. (1993), 74(3), 1310-19
 CODEN: JAPHEV; ISSN: 8750-7587

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effects of 3 chem. distinct protein kinase C activators on pulmonary vascular tone were studied in the buffer-perfused isolated rabbit lung. The 3 activators: 12-deoxyphorbol 13-isobutyrate (12,13-phorbol), mezerein, and 1-oleoyl-2-acetyl-sn-glycerol, produce concn.-dependent increases in pulmonary arterial pressure, whereas the inactive compd. 4.alpha.-phorbol 12,13-dibutyrate does not affect pulmonary arterial pressure. Reducing Ca availability with verapamil, a Ca-free buffer, or a chelator of intracellular Ca decreases the response to 12,13-phorbol or mezerein. Pretreatment with phloretin, an inhibitor of protein kinase C, has no affect on the vasoconstriction caused by infusion of a KCl bolus, but it does inhibit in a dose-dependent manner the response to 12,13-phorbol and mezerein. 12,13-Phorbol at a concn. of 2.5 .mu.M, but not of 1 .mu.M, stimulates prostacyclin and thromboxane synthesis by the

isolated lung. Because inhibitors of thromboxane synthesis decrease the response, thromboxane likely contributes to the vasoconstriction produced by higher concns. of 12,13-phorbol and mezerein. Pretreatment with isoproterenol or nitroprusside reduces the increase in pulmonary arterial pressure caused by the protein kinase C activators but does not reverse vasoconstriction, even though subsequent treatment with verapamil does. In summary: activating protein kinase C in the isolated rabbit lung causes long-lasting pulmonary vasoconstriction, reducing Ca availability decreases the response, part of the increase in pulmonary arterial pressure appears secondary to thromboxane generation, and pretreatment with isoproterenol or nitroprusside prevents the vasoconstriction, but posttreatment with these vasodilators is ineffective.

IT 34807-41-5, Mezerein

RL: BIOL (Biological study)

(lung vasoconstriction induction by, protein kinase C activation in relation to)

L58 ANSWER 25 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:143419 HCAPLUS

DOCUMENT NUMBER: 116:143419

TITLE: Different susceptibility of lung cell lines to inhibitors of tumor promotion and inducers of differentiation

AUTHOR(S): Zhu, H. G.; Tayeh, I.; Israel, L.; Castagna, M.

CORPORATE SOURCE: IRSC Lab., Villejuif, Fr.

SOURCE: J. Biol. Regul. Homeostatic Agents (1991), 5(2), 52-8

CODEN: JBRAER; ISSN: 0393-974X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Histolog. distinct lung tumor and normal cell lines were treated with a variety of potential inhibitors of cell growth such as inducers of cell differentiation, inhibitors of protein kinase C and inhibitors of tumor promotion. The response was assessed by [3H] thymidine incorporation and cloning efficiency. Both phorbol retinoate acetate and mezerein stimulated growth in lung normal cell lines (human fibroblastic PEH cells and rat epithelial TP9 cells) while inhibiting growth in lung tumor cell lines (human small-cell cancer-derived cell line IRSC-10M and adenocarcinoma-derived cell line A549). Likewise, the hydrophobic peptide melittin did not inhibit growth and cloning efficiency of normal cells at 1 .mu.M, a concn. which prevented proliferation in tumor cells. Protein kinase C inhibitors, chlorpromazine, trifluoperazine and 1-(5-isoquinolinyisulfonyl) 2-methylpiperazine, were much more effective on proliferation of IRSC-10M than of A549 cells. In contrast, the latter cells were more susceptible to anti-promoters such as glycyrrhetic acid, an antiinflammatory agent, and 3,4,2',4'-tetrahydroxychalcone or 2,3,5-trimethyl-6(12-hydroxy-5,10-dodecadiynyl)-1,4-benzoquinone, two inhibitors of lipxygenase, a key enzyme in arachidonate metab. These results provide evidence that small-cell carcinoma-derived cells, in contrast with adenocarcinoma-derived cells, are growth-inhibited by protein kinase C inhibitors and poorly dependent on the arachidonate metab. This difference in responsiveness suggests that different growth signalling pathways are preferentially triggered in these histol. distinct lung tumor cell lines. As a consequence, the proper susceptibility of tumor cells to phenotype modifiers has to be taken into account in cancer therapy.

IT 34807-41-5, Mezerein

RL: BIOL (Biological study)

(lung tumor cells of humans and lab. animals susceptibility to)

L58 ANSWER 26 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:120903 HCAPLUS

DOCUMENT NUMBER: 116:120903

TITLE: Use of a modulator of protein phosphorylation in the treatment of amyloidosis associated with Alzheimer's disease

INVENTOR(S): Buxbaum, Joseph D.; Gandy, Samuel E.; Greengard, Paul

PATENT ASSIGNEE(S): Rockefeller University, USA

SOURCE: Eur. Pat. Appl., 15 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 457295	A2	19911121	EP 1991-107844	19910515
EP 457295	A3	19920805		
EP 457295	B1	19970409		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 07025786	A2	19950127	JP 1991-136925	19910514
CA 2042668	AA	19911117	CA 1991-2042668	19910515
AT 151287	E	19970415	AT 1991-107844	19910515
ES 2102986	T3	19970816	ES 1991-107844	19910515

PRIORITY APPLN. INFO.: US 1990-524202 19900516

AB Disclosed is the use of .gtoreq.1 kinase modulator or phosphatase modulator capable of increasing or decreasing the rate of proteolytic processing of proteins found in intracellular neurofibrillary tangles and extracellular amyloid plaques for the prepn. of a pharmaceutical for the treatment of amyloidosis assocd. with Alzheimer's disease. The pharmaceutical contains the modulator in an amt. effectively regulating phosphorylation of the proteins.

IT 34807-41-5

RL: BIOL (Biological study)
(as kinase stimulator, for treatment of amyloidosis assocd. with
Alzheimer's disease)

L58 ANSWER 27 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:456233 HCAPLUS

DOCUMENT NUMBER: 113:56233

TITLE: Selective inactivation of peroxisomal and cytosolic 3-ketothiolase IB by 2-chloro-6-phenylhexanoate in intact hepatocytes

AUTHOR(S): Sephton, Gregory B.; Lowenstein, John M.

CORPORATE SOURCE: Grad. Dep. Biochem., Brandeis Univ., Waltham, MA, 02254-9110, USA

SOURCE: J. Biol. Chem. (1990), 265(16), 9214-20

CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Rat liver mitochondria and cytosol contain 2 types of 3-ketothiolases, namely 3-ketothiolases IA and IB, which cleave 3-ketoacyl-CoA (CoA) esters contg. .gtoreq.4 atoms and 3-ketothiolases IIA and IIB, which cleave 3-ketoacyl-CoA esters contg. 4 C atoms, i.e. acetoacetyl-CoA. Rat liver peroxisomes also contain 3-ketothiolases IA and IB and show that incubation of hepatocytes with 2-chloro-6-phenylhexanoate causes the selective inactivation of peroxisomal and cytosolic 3-ketothiolase IB,

whereas mitochondrial 3-ketothiolases are not appreciably affected. The basis of the selectivity of the inhibitor for peroxisomal and cytosolic 3-ketothiolases can be accounted for in terms of the specificities of the enzymes in the different pathways of β -oxidn. Evidence is presented that 2-chloro-6-phenylhexanoate is metabolized to 2-chloro-3-oxo-6-phenylhexanoyl-CoA, which then alkylates 3-ketothiolase and thereby inactivates the enzyme. Evidence is presented which suggests that cytosolic 3-ketothiolases IA and IB are not artifacts of homogenization and organelle prepn.

IT 128409-67-6

RL: BIOL (Biological study)
(ketothiolase of **liver** cytosol and peroxisome inhibition by)

IT 128409-68-7

RL: BIOL (Biological study)
(ketothiolase of **liver** cytosol and peroxisome inhibition by
chlorophenylhexanoate mediation by)

L58 ANSWER 28 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:147312 HCAPLUS

DOCUMENT NUMBER: 110:147312

TITLE: Effects of activators of protein kinase C, including bryostatins 1 and 2, on the growth of A549 human lung carcinoma cells

AUTHOR(S): Dale, Ian L.; Gescher, Andreas

CORPORATE SOURCE: Pharm. Sci. Inst., Aston Univ., Birmingham, B4 7ET, UK

SOURCE: Int. J. Cancer (1989), 43(1), 158-63

CODEN: IJCNAW; ISSN: 0020-7136

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Phorbol esters inhibit the growth of A549 human lung carcinoma cells at non-toxic concns., whereas 1-oleoyl-2-acetylgllycerol and 1,2-dioctanoylglycerol, synthetic analogs of the physiol. ligands of protein kinase C (PKC), do not. Expts. were conducted to test the hypothesis that other activators of PKC are capable of interfering with A549 cell growth. The non-phorboid tumor promoter mezerein mimicked the growth-inhibitory effect of TPA in that it arrested growth for 5 days, after which cells proliferated again in the presence of TPA. TPA was 20 times more potent as a growth inhibitor than mezerein. Bryostatin 1 at 10 nM and bryostatin 2 at 100 nM also arrested A549 cell growth and inhibited DNA replication as measured by incorporation of [Me-3H]-thymidine into cells. Inhibition of DNA synthesis to 75-90% of control values developed during the first hour of incubations of the cells with TPA, mezerein or bryostatins. The extent of inhibition changed little during the subsequent 5 h of incubation, after which it increased further to reach maximal values within 12 h. At concns. above those which caused maximal growth inhibition, the bryostatins abolished both their own inhibition of DNA synthesis and the anti-replicative effect of TPA and mezerein. Thus, activators of PKC other than phorbol esters are capable of inhibiting the growth of A549 cells. The bryostatins not only interfere with A549 cell growth but can also counter the growth-inhibitory effect of PKC activators, presumably via interaction with a target different from the phorbol ester receptor site.

IT 34807-41-5, Mezerein

RL: BIOL (Biological study)
(**lung** carcinoma growth of human inhibition by, as protein
kinase C activator)

L58 ANSWER 29 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:69933 HCAPLUS

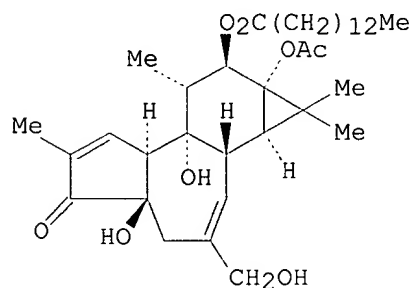
DOCUMENT NUMBER: 110:69933
 TITLE: Platelet-activating factor stimulates arachidonic acid metabolism in rat liver cells (C-9 cell line) by a receptor-mediated mechanism
 AUTHOR(S): Levine, Lawrence
 CORPORATE SOURCE: Dep. Biochem., Brandeis Univ., Waltham, MA, 02254, USA
 SOURCE: Mol. Pharmacol. (1988), 34(6), 793-9
 CODEN: MOPMA3; ISSN: 0026-895X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Platelet-activating factor (PAF) stimulated prodn. of PGI₂, PGE₂, and PGF₂.alpha., by rat liver cells (the C-9 cell line); as little as 0.2 nM PAF was effective. Enantio-PAF was 1000-fold less effective. Lyso-PAF, at 0.1-1.0 .mu.M, did not stimulate PGI₂ prodn. The synthesis of PGI₂ was essentially complete in 10 min. The stimulation by PAF of PGI₂ prodn. was inhibited by the PAF antagonists L 659989, kadsurenone, L 652731, and BN 52021; the values for 50% inhibition (IC₅₀) were 0.02, 0.19, 0.21, and 0.73 .mu.M, resp. The antagonists L 659989 and BN 52021 had no effect on the levels of 6-oxo-PGF₁.alpha. stimulated by TPA, palytoxin, melittin, the Ca²⁺ ionophore A 23187, colchicine, transforming growth factor .alpha., or exogenous arachidonic acid. The effect of PAF on arachidonic acid metab. was inhibited by prior exposure of the cells to PAF. Prior treatment of the rat liver cells at 37.degree. with the TPA-type tumor promoters TPA, teleocidin, and aplysiatoxin, as well as with the 2nd-stage tumor promoter mezerein, all of which activate the Ca²⁺/phospholipid-dependent protein kinase (protein kinase C), resulted not only in homologous desensitization to the TPA-type tumor promoters and mezerein, but also in heterologous desensitization to PAF. Stimulation of PGI₂ prodn. by palytoxin, A 23187, or exogenous arachidonic acid was not inhibited by such prior treatments with the TPA-type tumor promoters. Prior treatment of the cells at 37.degree. for 30 min with the non-TPA-type tumor promoters okadaic acid or palytoxin, both of which do not activate protein kinase C, did not result in heterologous desensitization to PAF.
 IT 34807-41-5, Mezerein
 RL: BIOL (Biological study)
 (liver cells desensitization to platelet-activating factor stimulation of prostaglandin formation by)

L58 ANSWER 30 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1988:586743 HCAPLUS
 DOCUMENT NUMBER: 109:186743
 TITLE: Construction of novel chiral synthons with enzymes and application to natural product synthesis. Part 23. Enantioselective hydrolysis of dialkyl 3-monosubstituted glutarates with pig liver esterase: structure-optical purity relationships
 AUTHOR(S): Nakada, Masahisa; Kobayashi, Susumu; Ohno, Masaji; Iwasaki, Shigeo; Okuda, Shigenobu
 CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan
 SOURCE: Tetrahedron Lett. (1988), 29(32), 3951-4
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 109:186743
 AB Dialkyl 3-monosubstituted glutarates are subjected to hydrolysis with pig liver esterase to afford the corresponding chiral half-esters. Synthetically useful half-esters of higher optical purity are obtained from the prochiral substrates of more hydrophobic nature.

IT 117213-93-1
 RL: RCT (Reactant)
 (enantioselective hydrolysis of, with pig liver esterase)

IT 117214-00-3P
 RL: PREP (Preparation)
 (prepn. of, from dialkyl glutarate enantioselective hydrolysis with pig liver esterase)

L58 ANSWER 31 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1988:126358 HCAPLUS
 DOCUMENT NUMBER: 108:126358
 TITLE: Differential effects of tumor promoters on the growth of normal human bronchial epithelial cells and human lung tumor cell lines
 AUTHOR(S): Sanchez, J. H.; Boreiko, C. J.; Furlong, J.; Hesterberg, T. W.
 CORPORATE SOURCE: Dep. Gen. Toxicol., Chem. Ind. Inst. Toxicol., Research Triangle Park, NC, 27709, USA
 SOURCE: Toxicol. In Vitro (1987), 1(4), 183-8
 CODEN: TIVIEQ; ISSN: 0887-2333
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

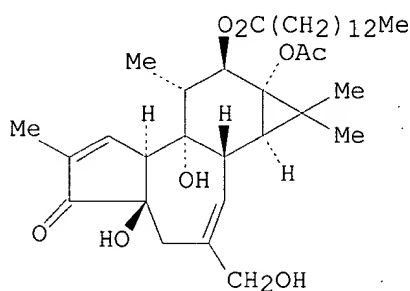


AB The effects of TPA (I) on the colony-forming efficiency and growth of normal human bronchial epithelial (NHBE) cells and 5 lung squamous carcinoma cell lines were compared in medium contg. 1% fetal bovine serum. TPA (0.1-5.0 ng/mL) inhibited the growth of NHBE cells and 1 carcinoma cell line, whereas 4 of the 5 carcinoma lines were less sensitive to the growth-inhibitory properties of TPA but were slightly inhibited at higher TPA concns. The responses of NHBE cells and carcinoma cells to TPA, and the related compds., mezerein, 4-O-Me TPA, and phorbol were then compared in serum-free medium. In general, the removal of serum from the medium increased the differences in the responses to TPA between normal and tumor cells. Two carcinoma lines inhibited by TPA in 1% serum were stimulated by TPA in the absence of serum. Mezerein and, to a lesser extent, 4-O-Me TPA also produced differential responses in colony-forming efficiencies between tumor lines and NHBE cells. Phorbol had no effect on either NHBE cells or on carcinoma cell lines. The relative insensitivity of carcinoma cell lines to the growth inhibitory effects of tumor promoters is consistent with the hypothesis that tumor promotion involves selection against normal cells to permit clonal expansion of preneoplastic or neo cell types.

IT 34807-41-5, Mezerein
 RL: BIOL (Biological study)

(colony-forming efficiency and growth of human bronchial epithelial cells and human **lung** tumor cell lines response to)

L58 ANSWER 32 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1986:124747 HCAPLUS
 DOCUMENT NUMBER: 104:124747
 TITLE: Novel serine phosphorylation of pp60c-src in intact cells after tumor promoter treatment
 AUTHOR(S): Gentry, Larry E.; Chaffin, Karen E.; Shoyab, Mohammed; Purchio, A. F.
 CORPORATE SOURCE: ONCOGEN, Seattle, WA, 98121, USA
 SOURCE: Mol. Cell. Biol. (1986), 6(2), 735-8
 CODEN: MCEBD4; ISSN: 0270-7306
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



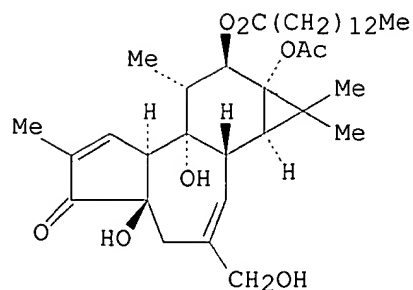
I

AB Treatment of normal cells with the tumor promoters TPA (I) [16561-29-8] and mezerein [34807-41-5] resulted in increased phosphorylation of the neoplastic-transforming protein pp60c-src. Two-dimensional tryptic phosphopeptide anal. of partial V8 protease fragments indicated that this phosphorylation takes place on a serine [56-45-1] residue and represents the major phosphorylation site following tumor promoter treatment. Untreated cells exhibited a low but detectable level of phosphorylation at this serine residue. The significance of these results with respect to the phosphoregulation of pp60c-src as well as tumor promotion is discussed.

IT **34807-41-5**

RL: BIOL (Biological study)
 (protein phosphorylation enhancement by, in **lung** cells)

L58 ANSWER 33 OF 47 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1986:124685 HCAPLUS
 DOCUMENT NUMBER: 104:124685
 TITLE: Effects of 12-O-tetradecanoylphorbol 13-acetate on adhesiveness and lung-colonizing ability of Lewis lung carcinoma cells
 AUTHOR(S): Takenaga, Keizo; Takahashi, Katsuhiko
 CORPORATE SOURCE: Dep. Chemother., Chiba Cancer Cent. Res. Inst., Chiba, 280, Japan
 SOURCE: Cancer Res. (1986), 46(1), 375-80
 CODEN: CNREA8; ISSN: 0008-5472
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



I

AB The potent tumor promoter 12-O-tetradecanoylphorbol 13-acetate (TPA) (I) [16561-29-8] enhanced the adherence of low-metastatic Lewis **lung** carcinoma cells (P-29) to the surface of plastic culture dishes and to monolayers of endothelial cells. This effect was transient, being apparent within 15 min and maximal within 1 h after treatment with TPA. Biol. active analogs of TPA and mezerein [34807-41-5] also enhanced attachment of P-29 cells, whereas inactive analogs of TPA did not. TPA-treated P-29 cells formed many more pulmonary nodules than did untreated P-29 cells when injected i.v. into C57BL/6 mice. The kinetics of enhancement of attachment of P-29 cells after TPA treatment coincided well with that of enhancement of their **lung**-colonizing ability. Addn. of TPA to P-29 cells stimulated phosphorylation of a cellular protein with a mol. wt. of 54,000. The possibility that this phosphorylation was related to activation of Ca-phospholipid-dependent protein kinase was suggested by the fact that phospholipid breakdown induced by exogenous treatment of the cells with *Clostridium perfringens* phospholipase C [9001-86-9] and 1-oleoyl-2-acetyl-glycerol [84746-00-9] also enhanced Mr 54,000 cellular protein phosphorylation. However, neither phospholipase C nor 1-oleoyl-2-acetyl-glycerol enhanced attachment of P-29 cells or their **lung**-colonizing ability.

IT 34807-41-5

RL: BIOL (Biological study)
(**lung** carcinoma cell adhesiveness and **lung**
colonizing ability response to pretreatment with)

L58 ANSWER 34 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:144549 HCAPLUS

DOCUMENT NUMBER: 102:144549

TITLE: Response of cultured rat liver epithelial cell lines to tumor-promoting phorbol esters

AUTHOR(S): Ljubimov, Alexander V.; Martel, Nicole; Yamasaki, Hiroshi

CORPORATE SOURCE: Int. Agency Res. Cancer, Lyon, 69372, Fr.

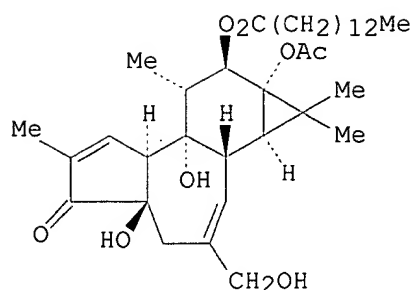
SOURCE: Exp. Cell Res. (1985), 156(2), 311-26

CODEN: ECREAL; ISSN: 0014-4827

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The membrane effects of a potent tumor promoter, TPA (I) [16561-29-8], were studied in a series of cultured rat liver epithelial cell lines. Treatment with TPA resulted in the formation of strand-like aggregates (ridges) of viable cells over the monolayer of IAR 6-1 cells, but not of 3 other cell lines tested (IAR 20, IAR 6, IAR 6-7). A class of specific, saturable, high-affinity receptors for phorbol esters was demonstrated in all 4 cell lines employing a conventional 20-3H-labeled phorbol 12,13-dibutyrate [37558-16-0]-binding assay. The dissociation constants were similar in 4 lines, but the number of receptors per cell in IAR 6-1 cells was about twice that in other lines. Down-regulation of receptors was demonstrated in IAR 20 and IAR 6-1 cells with similar characteristics. Iodinable surface proteins and galactose-containing surface glycoproteins did not respond to TPA. The distribution of fibronectin, laminin-entactin, and procollagen type III was not affected by TPA. A TPA-responsive cell line, IAR 6-1, contained considerably less laminin-entactin than did the other lines. TPA had no influence on metabolic labeling of 3H-labeled fucose-containing cellular glycoprotein in IAR 6-1 cells. One specific protein, with molecular mass of 78 kdaltons was more heavily labeled in IAR 6-1 cells than in the other cell lines. The responsive cells (IAR 6-1) differed from nonresponsive ones in having more phorbol ester receptors, increased fucosylation of a specific glycoprotein, and decreased deposition of laminin-entactin in the extracellular matrix.

IT 34807-41-5

RL: PROC (Process)

(binding of, by receptors of cultured liver epithelial cells)

L58 ANSWER 35 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:2495 HCAPLUS

DOCUMENT NUMBER: 102:2495

TITLE: Mechanism of inactivation of chymotrypsin by 3-benzyl-6-chloro-2-pyrone

AUTHOR(S): Gelb, Michael H.; Abeles, Robert H.

CORPORATE SOURCE: Grad. Dep. Biochem., Brandeis Univ., Waltham, MA, 02254, USA

SOURCE: Biochemistry (1984), 23(26), 6596-604

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The mechanism of inactivation of chymotrypsin (I) by 3-benzyl-6-chloro-2-pyrone was studied. Chloride analog of inactivated I suggested that the complex did not contain intact chloropyrone or an acid chloride. ¹³C NMR studies of I inactivated with ¹³C-enriched chloropyrones showed that (1) the pyrone ring was no longer intact, (2) C-6 became a carboxylate group and C-2 became esterified to the enzyme, probably to serine-195, and (3) a double bond was present adjacent to the serine ester. Inactivated I

slowly regained catalytic activity with the concomitant release of (E)-4-benzyl-2-pentenedioic acid. Evidently, double bond migration occurred during reactivation, since the position of the double bond in the released diacid product was different than in the inactivator-enzyme complex. When the reactivation was carried out in $[18O]H_2O$ -enriched water, a single 18O was incorporated into the released product, and this was further evidence that the inactivator is bound to the enzyme only through a single ester linkage. A 2H isotope effect on reactivation was obsd. when a chloropyrone deuterated at C-5 was used. Thus, removal of a proton from C-5 is required for reactivation, and isomerization of the double bond and not hydrolysis of the acyl-enzyme is rate detg. A variety of amines accelerated the rate of reactivation by functioning as general bases and not as nucleophiles. A reaction scheme is presented that accounts for the formation of the stable inactivator-enzyme complex as well as the prodn. of 2 products derived from enzymic hydrolysis of the chloropyrone. The importance of a C-6-derived carboxylate group in the stabilization of the acyl-enzyme is discussed.

IT 85533-88-6

RL: FORM (Formation, nonpreparative)
(formation of, from benzylchloropyrone by **chymotrypsin**,
enzyme inactivation in relation to)

IT 93383-65-4

RL: FORM (Formation, nonpreparative)
(formation of, in benzylchloropyrone inactivation of
chymotrypsin)

L58 ANSWER 36 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:134019 HCAPLUS

DOCUMENT NUMBER: 100:134019

TITLE: Effects of tumor promoters on the frequency of
metallothionein I gene amplification in cells exposed
to cadmium

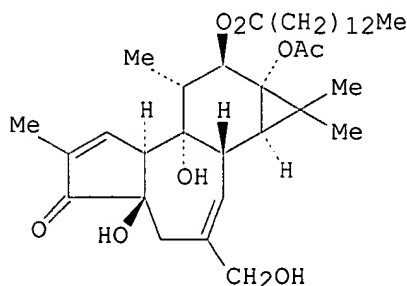
AUTHOR(S): Hayashi, Kenshi; Fujiki, Hirota; Sugimura, Takashi
CORPORATE SOURCE: Biochem. Div., Natl. Cancer Cent. Res. Inst., Tokyo,
104, Japan

SOURCE: Cancer Res. (1983), 43(11), 5433-6
CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Three potent tumor promoters of different classes, 12-O-tetradecanoylphorbol 13-acetate (I) [16561-29-8], dihydroteleocidin B

[7491-76-1] and aplysiatoxin [52659-57-1], and 2 moderate tumor promoters, mezerein [34807-41-5], and debromoaplysiatoxin [52423-28-6], enhanced the frequency of appearance of Cd-resistant Chinese hamster lung cells when the cells were exposed to cytotoxic levels of CdCl₂. With these compds., the activity to induce Cd-resistant cells correlated well with the potency of tumor-promoting activity. Cd resistance, which persisted after removal of the tumor promoters, was assocd. with the overprodn. of metallothionein I mRNA. The amplified metallothionein I genes were shown by Southern blotting expts. The relevance of the gene amplification caused by tumor promoters is discussed in relation to cancer development and progression.

L58 ANSWER 37 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:115151 HCAPLUS

DOCUMENT NUMBER: 100:115151

TITLE: Long-acting contraceptive agents: in vitro hydrolysis of esters of norethisterone and levonorgestrel

AUTHOR(S): Naderi, S.; Fotherby, K.

CORPORATE SOURCE: Dep. Steroid Biochem., R. Postgrad. Med. Sch., London, W12 0HS, UK

SOURCE: Steroids (1983), 41(3), 397-417

CODEN: STEDAM; ISSN: 0039-128X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Hydrolysis of 108 norethisterone esters and 49 levonorgestrel esters by rabbit liver was studied in vitro. For straight chain esters, introduction of a triple or double bond at C4, C5, or C6 did not inhibit hydrolysis; however, a decrease in hydrolysis was produced by replacement of a methylene group by an O atom. Except for short chain esters, hydrolysis was inhibited by substituents at C2 of the ester chain. Cyclopropylcarboxylate and cyclobutylcarboxylate were readily hydrolyzed, and introduction of a furan ring into the side chain did not affect hydrolysis. Cholesteryl carbonate ester and pentamethyldisilyloxy ether were not hydrolyzed by the liver prepn. Levonorgestrel esters were hydrolyzed more slowly than norethisterone esters, and biol. potency of the esters was independent of the rate of hydrolysis in vitro. Apparently, hydrolysis rate is not the major factor involved in expression of biol. activity, with uptake from the injection site probably being more important.

IT 89094-62-2 89094-76-8

RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(hydrolysis of, by liver)

L58 ANSWER 38 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:418590 HCAPLUS

DOCUMENT NUMBER: 99:18590

TITLE: Novel inactivators of serine proteases based on 6-chloro-2-pyrone

AUTHOR(S): Westkaemper, Richard B.; Abeles, Robert H.

CORPORATE SOURCE: Grad. Dep. Biochem., Brandeis Univ., Waltham, MA, 02254, USA

SOURCE: Biochemistry (1983), 22(13), 3256-64

CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The interaction of serine protease (esterases) with 6-chloro-2-pyrones was investigated. Time-dependent inactivation of chymotrypsin, .alpha.-lytic protease, pig liver elastase, and acetylcholinesterase was found with 3- and 5-benzyl-6-chloro-2-pyrone, as well as 3- and 5-methyl-6-chloro-2-

pyrone. No inactivation was obsd. with the unsubstituted 6-chloro-2-pyrone. The substituted pyrones did not inactivate papain or carboxypeptidase A, nor a no. of other nonproteolytic enzymes. The substituted chloropyrones, therefore, show considerable selectivity toward serine proteases. Analogs in which the 6-chloro substituent is replaced by H or OH do not inactivate. The presence of the halogen is, therefore, essential for inactivation. Chymotrypsin catalyzes the hydrolysis of 3-benzyl-6-chloro-2-pyrone. At pH 7.5, (E)-4-benzyl-2-pentenedioic acid is the major product, and 2-benzyl-2-pentenedioic anhydride is a minor product. The ratio of hydrolysis product found to the no. of enzyme mols. inactivated varies in the range 14-40. The enzyme inactivated with the 3-benzyl compd. does not show a spectrum characteristic of the pyrone ring. This suggests that inactivation by 3-benzyl-6-chloro-2-pyrone occurs in a mechanism-based fashion after enzymic lactone hydrolysis. When the enzyme is inactivated with the 5-benzyl compd., absorbance due to the pyrone ring is obsd. It is suggested that inactivation occurs through an active site directed mechanism involving a 1,6-conjugate addn. of an active site nucleophile to the pyrone ring.

IT 85533-83-1

RL: FORM (Formation, nonpreparative)
(formation of, in **chymotrypsin** reaction with benzylchloropyrone)

IT 85533-84-2 85533-85-3

RL: FORM (Formation, nonpreparative)
(formation of, in **chymotrypsin** reaction with benzylpentenedioic anhydride)

IT 85533-91-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with **chymotrypsin**)

L58 ANSWER 39 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:1508 HCAPLUS

DOCUMENT NUMBER: 98:1508

TITLE: Diversity of nuclear phorbol ester tumor promoter receptors in mouse liver: evidence for two classes of binding sites

AUTHOR(S): Perrella, Frank W.; Bussell, Pauline A.; Boutwell, R. K.

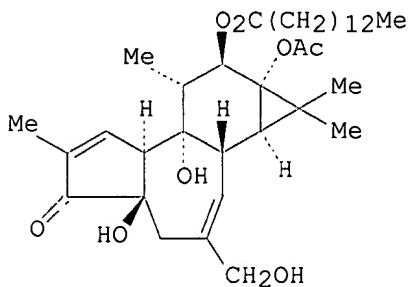
CORPORATE SOURCE: McArdle Lab. Cancer Res., Univ. Wisconsin, Madison, WI, 53706, USA

SOURCE: Biochem. Biophys. Res. Commun. (1982), 108(4), 1722-7
CODEN: BBRCA9; ISSN: 0006-291X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Two classes of phorbol ester binding sites were demonstrated in the nuclear fraction of liver from female CD-1 mice. Equil. binding studies of 0.40 M NaCl nuclear exts. yielded a sigmoidal satn. curve which was resolved by Hill plot anal. into 2 components. However, when nuclei were extd. in 0.24 M NaCl, the 12-O-tetradecanoylphorbol 13-acetate (I) [16561-29-8] satn. curve of the ext. was biphasic in the shape of both high and low affinity binding sites termed Class I and II receptors. When the 0.24 M NaCl extd. nuclear pellet was extd. further in 0.40 M NaCl, satn. anal. of the ext. revealed only the low affinity binding site (Class II). This is the 1st study to identify the existence of phorbol ester receptors in liver nuclei.

IT **34807-41-5**

RL: PRP (Properties)

(binding sites of, in **liver**, classes of)

L58 ANSWER 40 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:491946 HCAPLUS

DOCUMENT NUMBER: 97:91946

TITLE: Carboxylic acids

PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 57014555	A2	19820125	JP 1980-88477	19800701

OTHER SOURCE(S): CASREACT 97:91946

AB Thirty-four carboxylic acids $R_1C_6H_4C_6H_5-nR_n$ [I, = (carboxy) alkenylene or alkadienylene; R = substituted alkyl, alkenyl, aryl, etc.; $R_1 = CO_2H$, (carboxy) alkyl; n = 0-3] were prepd. by reaction of $R_nC_6H_5-nX_1CHO$ ($X_1 =$ alkylenylene, alkenylene) with $R_1C_6H_5(CH_2)_mCO_2H$ (m = 1-3). Liver function improving test data of I were given in rats using Congo Red. Thus, refluxing a mixt. of 0.94 g trans-PhCH:CHCHO, 0.9 g 3-HO₂CC₆H₄CH₂CO₂H, 1.1 mL Ac₂O, and 0.58 mL Et₃N 35 min gave 0.8 g (E,E)-3-HO₂CC₆H₄C(CO₂H):CHCH:CHPh.

IT **81995-43-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, for **liver** function improvement)

L58 ANSWER 41 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:418803 HCAPLUS

DOCUMENT NUMBER: 97:18803

TITLE: The role of free oxygen radicals in tumor promotion and carcinogenesis

AUTHOR(S): Troll, Walter; Witz, Gisela; Goldstein, Bernard; Stone, Donna; Sugimura, Takashi

CORPORATE SOURCE: Med. Cent., New York Univ., New York, NY, 10016, USA

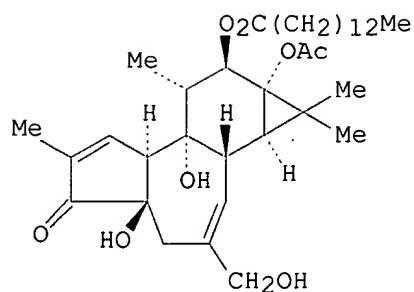
SOURCE: Carcinog. - Compr. Surv. (1982), 7(Cocarcinog. Biol. Eff. Tumor Promoters), 593-7

CODEN: CCSUDL; ISSN: 0147-4006

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB The formation of superoxide by polymorphonuclear lymphocyte (PMNs) was stimulated by phorbol 12-myristate 13-acetate (I) [16561-29-8], mezerein [34807-41-5], and teleocidin B [11032-05-6] which are tumor promoters. However, phorbol esters which are not tumor promoters did not enhance superoxide formation. Soybean and lima bean **trypsin** inhibitor [36357-77-4], retinol [68-26-8], retinyl acetate [127-47-9], retinoic acid [302-79-4] and other protease inhibitors inhibited the I-stimulated superoxide formation in PMNs. Probably, the free superoxide is responsible for the tumor promoter-induced cell damage.

L58 ANSWER 42 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:104596 HCAPLUS

DOCUMENT NUMBER: 96:104596

TITLE: Synthesis and properties of liquid crystals. III. Cholesterol esters of some cis-, trans-isomers of unsaturated acids

AUTHOR(S): Bogatskii, A. V.; Galatina, A. I.; Derkach, L. G.; Taubert, D.

CORPORATE SOURCE: Fiz.-Khim. Inst., Odessa, USSR

SOURCE: Zh. Org. Khim. (1981), 17(11), 2320-3

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The esters of cholesterol with cis- and trans-RCX:CHCO₂H (R = Me, Ph; X = H; R = Me, X = Cl) and with .alpha.-cis-.gamma.-trans- and .alpha.-trans-.gamma.-trans-RCH:CHCH:CHCO₂H (R = Me, Ph) were prepd. and their crystal .fwdarw. cholesteric mesophase, (T₁), cholesteric mesophase .fwdarw. isotropic liq. (T₂), and cholesteric mesophase .fwdarw. crystal transition temps. detd. The double bonds in the acid moiety facilitate formation of the cholesteric mesophase and retard crystn. Both T₁ and T₂ are higher for the trans than for the cis isomers. The Cl atom lowers the thermal stability of the cholesteric mesophase.

IT 28010-12-0 28010-13-1

RL: RCT (Reactant)

(esterification of, with **cholesterol**)

L58 ANSWER 43 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1978:16047 HCAPLUS

DOCUMENT NUMBER: 88:16047

TITLE: Effect of .beta.-benzalbutyramide on cholesterol biosynthesis

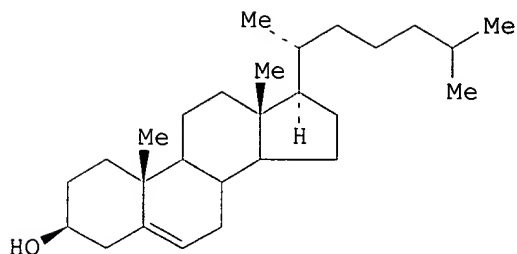
AUTHOR(S): Nakamura, Haruo

CORPORATE SOURCE: Dep. Oral Physiol., Hokkaido Univ. Sch. Dent., Sapporo, Japan

SOURCE: Igaku To Seibutsugaku (1976), 92(5), 421-3

DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: IGSBAL
Journal
Japanese



II

AB Administration of .beta.-benzalbutyramide (I) [7236-47-7] (100 mg/Kg) lowered plasma **cholesterol** (II) [57-88-5] in male rats given Triton WR 1339 (200 mg/Kg). II biosynthesis from acetate and mevalonate by **liver** was inhibited by I in vitro and in vivo. I inhibited the incorporation of mevalonate more markedly than that of acetate.

IT 7236-47-7

RL: BIOL (Biological study)
(**cholesterol** formation by **liver** inhibition by)

L58 ANSWER 44 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:150586 HCAPLUS

DOCUMENT NUMBER: 86:150586

TITLE: Effect of hypolipidemic and hypoglycemic drugs on ethanol induced hypertriglyceridemia in rats

AUTHOR(S): Puglisi, L.; Caruso, V.; Conti, F.; Fumagalli, R.; Sirtori, C.

CORPORATE SOURCE: Inst. Pharmacol. Pharmacogn., Univ. Milano, Milan, Italy

SOURCE: Pharmacol. Res. Commun. (1977), 9(1), 71-7

CODEN: PLRCAT

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An exptl. model of hypertriglyceridemia induced by subacute ethanol [64-17-5] administration was developed in rats. A four day schedule of administration induced a 50-100% increase of serum triglycerides, without changes in **cholesterol** levels. Drugs effective on lipid or glucose metab. were tested in this model. Hypoglycemic sulphonylureas, nicotinic acid, clofibrate, and the new hypolipidemic agent .beta.-benzalbutyrate diethylamide (C11) [58458-55-2] were effective agents in controlling ethanol induced hypertriglyceridemia. The activity of C11 was also confirmed in ethanol-induced hypertriglyceridemia in human volunteers.

L58 ANSWER 45 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1974:11894 HCAPLUS

DOCUMENT NUMBER: 80:11894

TITLE: Manipulation of enzyme function

AUTHOR(S): Fink, Gerhard; Thoma, Hans

CORPORATE SOURCE: Inst. Tech. Chem., Tech. Univ. Muenchen, Munich, Ger.

SOURCE: DECHEMA (Deut. Ges. Chem. Apparatew.) Monogr. (1973),

71, 295-314
CODEN: DMDGAG

DOCUMENT TYPE: Journal
LANGUAGE: German

AB Me cinnamoylacetate (PhCH:CHCOCH₂CO₂Me) (I) was synthesized as model substrate for chymotrypsin, as well as the p-methoxy derivs., Me 5-(p-methoxyphenyl)-3-ketovaleate, and Me 4-phenylbutadienecarboxylate. Only I was hydrolyzed by the enzyme. The rate was measured by the pH-stat method and was proportional to enzyme concn., with the greatest activity at pH 8. Substrate saturation occurred at 3.1 .times. 10⁻³M. There was no hydrolysis in the absence of enzyme. The model substrates were only slightly soluble in water, so MeOH, EtOH, dioxane, and Me₂SO were used as solvents. These solvents reduced the activity of the enzyme. The effect of these solvents was detd. on the chymotrypsin attached to CM-methylcellulose. The dioxane and Me₂SO systems gave the highest enzymic activity. The chymotrypsin was bound to the CM-cellulose by the azide method. N-Succinyl-L-phenylalanine- (SPNA), N-glutaryl-L-phenylalanine- (GPNA), N-acetyl-L-tyrosine- (ATNA), and L-phenylalanine- (PNA) p-nitroanilides were used as substrates in the column reactor and the rate of the reaction measured by the p-nitroaniline formed measured at 405 nm. When the amt. of product formation was plotted against time a break was found in the curve and the break was dependent on substrate and enzyme concn., but was independent of the flow rate of substrate soln. through the column. The charge on the CM-cellulose displaced the pH optimum of the reaction to 9.3. NaCl had a complex effect on the immobilized enzyme. Temp. effects on the immobilized enzyme were measured and the heat of reaction calcd. for the various substrates: ATNA, 15.6 Kcal/mole; GPNA, 15.5 kcal/mole and PNA, 14.2 kcal/mole.

IT 1516-24-1

RL: RCT (Reactant)
(reaction of, with **chymotrypsin**, kinetics of)

L58 ANSWER 46 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1972:471959 HCAPLUS

DOCUMENT NUMBER: 77:71959

TITLE: Specific modification of methionine-192 of .alpha.-chymotrypsin by an affinity label exploiting the orienting properties of the linear acetylenic group

AUTHOR(S): Jones, J. Bryan; Hysert, David W.

CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, Ont., Can.

SOURCE: Biochemistry (1972), 11(14), 2726-33

CODEN: BICHAW

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The practicability of incorporating acetylenic bonds into affinity labels in order to exploit their rodlike properties for improving the orientation of an alkylating function toward a selected protein nucleophile was demonstrated by the facile irreversible inhibition of .alpha.-chymotrypsin by 6-bromo-1-phenylhex-4-yn-3-one. 6-Bromo-1-phenylhex-4-yn-3-one was designed to achieve optimum orientation of its propargylic bromide alkylating function toward both histidine-57 and methionine-192. However, the latter function was alkylated selectively owing to its 100-fold greater reactivity with propargylic bromides. Rate of inhibition, pH-rate profile, competitive inhibition, effect on K_m(app) and k₃, amino acid anal., and diagonal peptide-mapping studies established that 6-bromo-1-phenylhex-4-yn-3-one was a methionine-192-specific, active-site-directed, irreversible inhibitor. The calcd. values of its K_i (10mM) and rate of inhibition const. (2.8 .times. 10⁻³ sec⁻¹) show it to

be one of the best methionine-192 of .alpha.-chymotrypsin directed affinity labels yet evaluated.

IT 37566-49-7

RL: BIOL (Biological study)
(**chymotrypsin** inhibition by, kinetics of)

L58 ANSWER 47 OF 47 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1969:113584 HCAPLUS

DOCUMENT NUMBER: 70:113584

TITLE: Inhibition of liver cholesterol biosynthesis by butyric acid derivatives

AUTHOR(S): Giorgini, D.; Porcellati, Giuseppe

CORPORATE SOURCE: Univ. Pavia, Pavia, Italy

SOURCE: Farmaco, Ed. Sci. (1969), 24(4), 392-401

CODEN: FRPSAX

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Previous work on cholesterol synthesis inhibition by various phenyl derivs. is reviewed. Exptl. evidence is reported which shows that cholesterol synthesis from labeled acetate in rat liver slices is markedly inhibited in vitro by .beta.-benzalbutyric acid, and in a less evident way also by .alpha.-hydroxy-.beta.-benzalbutyric acid. Cholesterol formation from labeled mevalonate is, on the contrary, scarcely affected under similar conditions by both compds. Results are also shown which indicate that a similar inhibition is brought about also by .beta.-benzalbutyramide in rat liver purified microsomes, supplemented by its supernatant fraction. Inhibition is similarly evident from acetate but is hardly present, when acetate is replaced by mevalonate. Expts. carried out with partially purified enzymes (acetate:CoA ligase, E.C. 6.2.1.1, and acetyl CoA-acetyl transferase, E.C. 2.3.1.9) show that only the 1st enzyme is inhibited in vitro by .beta.-benzalbutyric acid, although at concns. higher than those shown to be able to inhibit cholesterol formation by the slices. Suggestion is made that other enzymes of the acetate-mevalonate pathway might be inhibited in vitro by .beta.-benzalbutyric acid and its derivs.

IT 7236-47-7

RL: BIOL (Biological study)
(**cholesterol** formation by **liver** in response to)

=> select hit rn l58 1-47
E10 THROUGH E56 ASSIGNED

=> fil reg

FILE 'REGISTRY' ENTERED AT 14:29:59 ON 08 MAY 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 6 MAY 2002 HIGHEST RN 412003-61-3

DICTIONARY FILE UPDATES: 6 MAY 2002 HIGHEST RN 412003-61-3

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

=>

=> d his 159

(FILE 'HCAPLUS' ENTERED AT 14:29:01 ON 08 MAY 2002)
 SELECT HIT RN L58 1-47

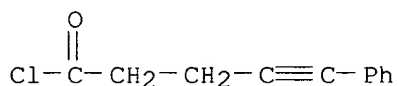
FILE 'REGISTRY' ENTERED AT 14:29:59 ON 08 MAY 2002
 L59 47 S E10-E56

=>

=>

=> d ide can 159 1-47

L59 ANSWER 1 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 300662-69-5 REGISTRY
 CN 4-Pentynoyl chloride, 5-phenyl- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C11 H9 Cl O
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT

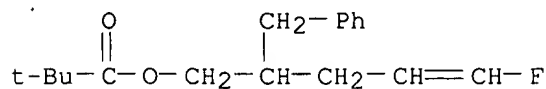


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:296331

L59 ANSWER 2 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 205373-53-1 REGISTRY
 CN Propanoic acid, 2,2-dimethyl-, 5-fluoro-2-(phenylmethyl)-4-pentenyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C17 H23 F O2
 SR CA
 LC STN Files: CA, CAPLUS

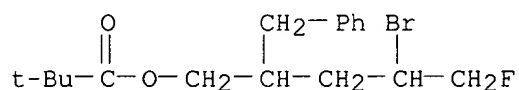


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:291977

L59 ANSWER 3 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 205373-49-5 REGISTRY
 CN Propanoic acid, 2,2-dimethyl-, 4-bromo-5-fluoro-2-(phenylmethyl)pentyl
 ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C17 H24 Br F O2
 SR CA
 LC STN Files: CA, CAPLUS

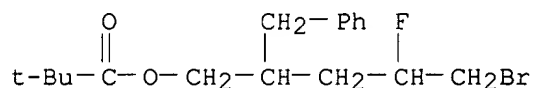


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:291977

L59 ANSWER 4 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 205373-47-3 REGISTRY
 CN Propanoic acid, 2,2-dimethyl-, 5-bromo-4-fluoro-2-(phenylmethyl)pentyl
 ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C17 H24 Br F O2
 SR CA
 LC STN Files: CA, CAPLUS



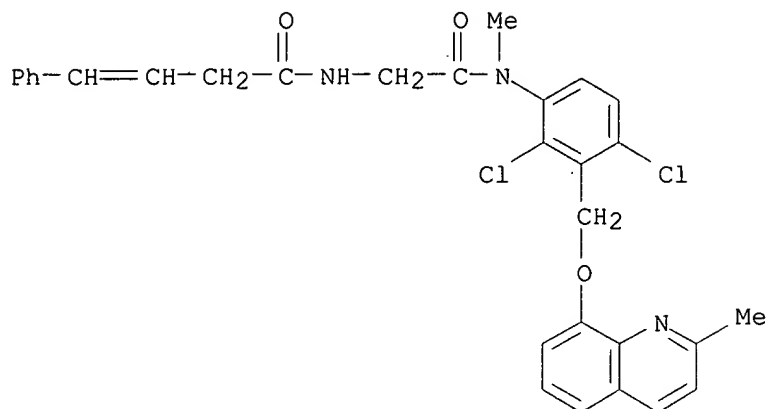
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1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:291977

L59 ANSWER 5 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 199791-52-1 REGISTRY
 CN 3-Butenamide, N-[2-[[2,4-dichloro-3-[(2-methyl-8-quinolinyl)oxy]methyl]phenyl]methylamino]-2-oxoethyl]-4-phenyl- (9CI) (CA INDEX NAME)
 FS 3D CONCORD

MF C30 H27 Cl2 N3 O3
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:30416

REFERENCE 2: 128:30415

L59 ANSWER 6 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN **180728-05-6** REGISTRY

CN Carbamic acid, [3-[[[(4-aminophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethylene)propyl]-, tetrahydro-3-furanyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

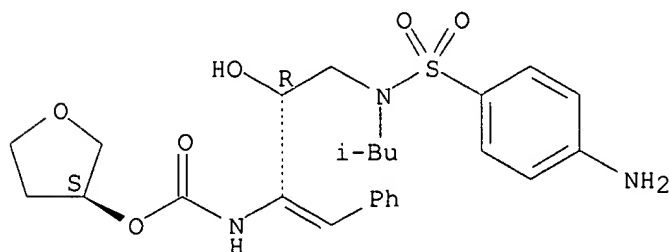
FS STEREOSEARCH

MF C25 H33 N3 O6 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.
 Double bond geometry unknown.



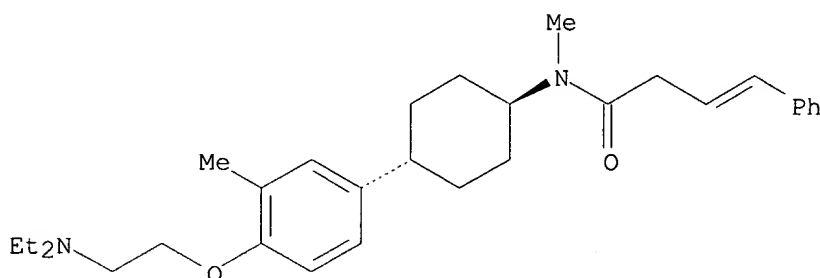
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:184776

L59 ANSWER 7 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN 178541-89-4 REGISTRY
CN 3-Butenamide, N-[4-[4-[2-(diethylamino)ethoxy]-3-methylphenyl]cyclohexyl]-
N-methyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H42 N2 O2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.
Double bond geometry unknown.



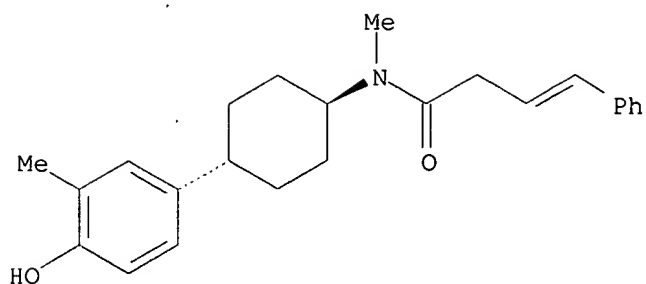
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1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:86319

L59 ANSWER 8 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN 178541-15-6 REGISTRY
CN 3-Butenamide, N-[4-(4-hydroxy-3-methylphenyl)cyclohexyl]-N-methyl-4-phenyl-,
trans- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H29 N O2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:86319

L59 ANSWER 9 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 178540-64-2 REGISTRY

CN 3-Butenamide, N-methyl-4-phenyl-N-[4-(5-pyrimidinyl)cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

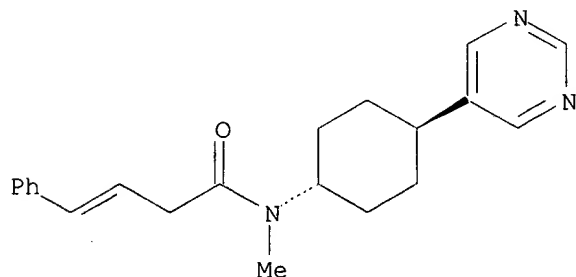
MF C21 H25 N3 O

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.

Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:86319

L59 ANSWER 10 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 178540-37-9 REGISTRY

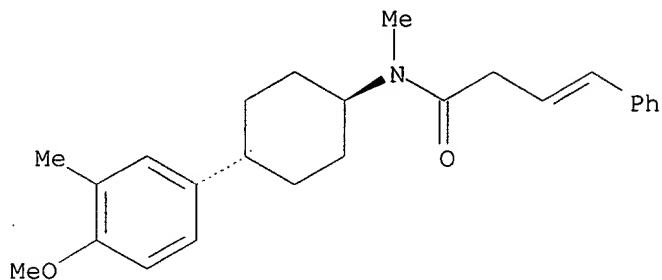
CN 3-Butenamide, N-[4-(4-methoxy-3-methylphenyl)cyclohexyl]-N-methyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H31 N O2

SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.
Double bond geometry unknown.



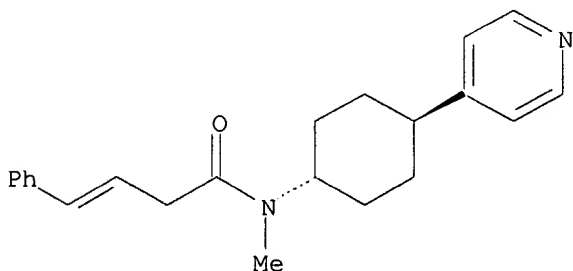
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:86319

L59 ANSWER 11 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN 178540-24-4 REGISTRY
CN 3-Butenamide, N-methyl-4-phenyl-N-[4-(4-pyridinyl)cyclohexyl]-, trans-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H26 N2 O
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

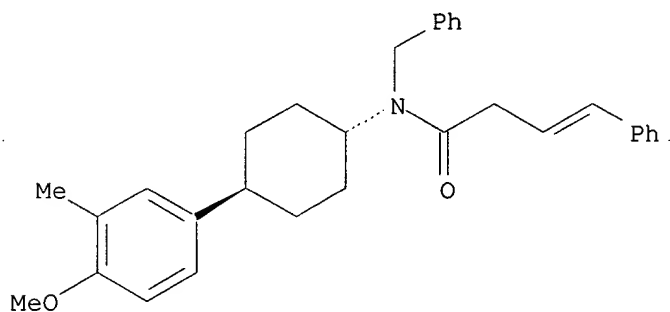
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:86319

L59 ANSWER 12 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 178365-08-7 REGISTRY
 CN 3-Butenamide, N-[4-(4-methoxy-3-methylphenyl)cyclohexyl]-4-phenyl-N-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C31 H35 N O2
 SR CA
 LC STN Files: CA, CAPLUS

Relative stereochemistry.
 Double bond geometry unknown.



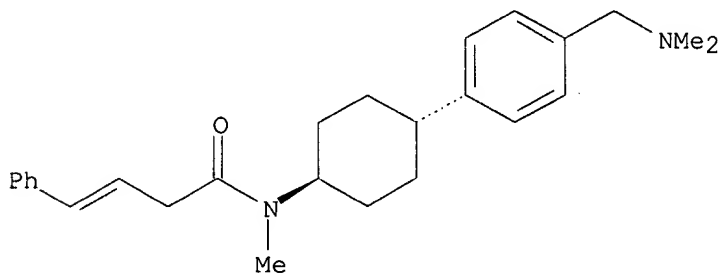
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1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:58115

L59 ANSWER 13 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 178163-33-2 REGISTRY
 CN 3-Butenamide, N-[4-[4-[(dimethylamino)methyl]phenyl]cyclohexyl]-N-methyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C26 H34 N2 O
 SR CA
 LC STN Files: CA, CAPLUS

Relative stereochemistry.
 Double bond geometry unknown.



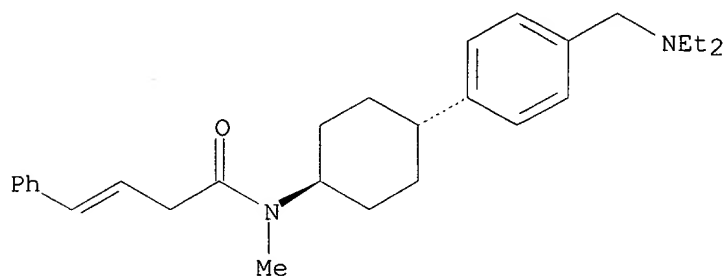
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1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:58083

L59 ANSWER 14 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 178162-88-4 REGISTRY
 CN 3-Butenamide, N-[4-[4-[(diethylamino)methyl]phenyl]cyclohexyl]-N-methyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C28 H38 N2 O
 SR CA
 LC STN Files: CA, CAPLUS

Relative stereochemistry.
 Double bond geometry unknown.



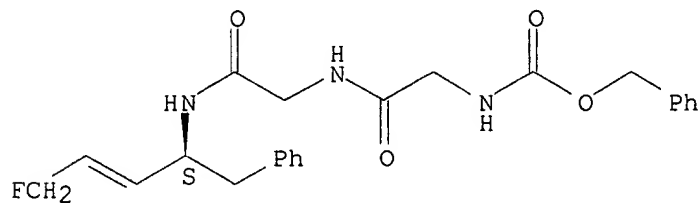
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:58083

L59 ANSWER 15 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 173866-73-4 REGISTRY
 CN Glycinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[4-fluoro-1-(phenylmethyl)-2-butenyl]-, (S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C23 H26 F N3 O4
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.
 Double bond geometry unknown.



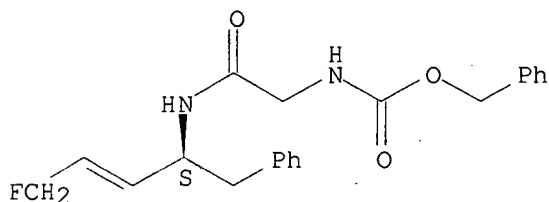
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1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 16 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN **173866-72-3** REGISTRY
CN Carbamic acid, [2-[[4-fluoro-1-(phenylmethyl)-2-butenyl]amino]-2-oxoethyl]-
phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H23 F N2 O3
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



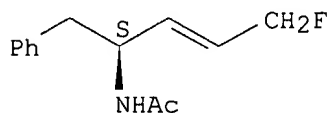
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 17 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN **173866-71-2** REGISTRY
CN Acetamide, N-[4-fluoro-1-(phenylmethyl)-2-butenyl]-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C13 H16 F N O
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 18 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 173866-70-1 REGISTRY

CN Glycinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[4-chloro-1-(phenylmethyl)-2-butenyl]-, (S)- (9CI) (CA INDEX NAME)

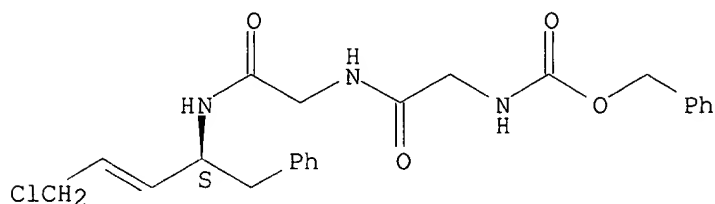
FS STEREOSEARCH

MF C23 H26 Cl N3 O4

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 19 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 173866-69-8 REGISTRY

CN Glycinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[4-bromo-1-(phenylmethyl)-2-butenyl]-, (S)- (9CI) (CA INDEX NAME)

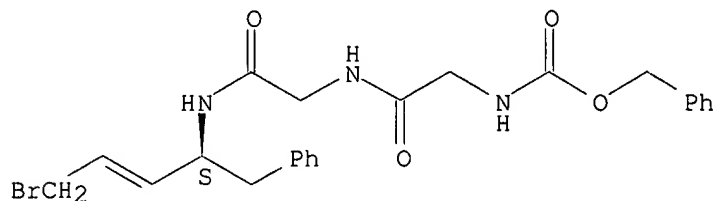
FS STEREOSEARCH

MF C23 H26 Br N3 O4

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 20 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 173866-68-7 REGISTRY

CN Carbamic acid, [2-[[4-chloro-1-(phenylmethyl)-2-butenyl]amino]-2-oxoethyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

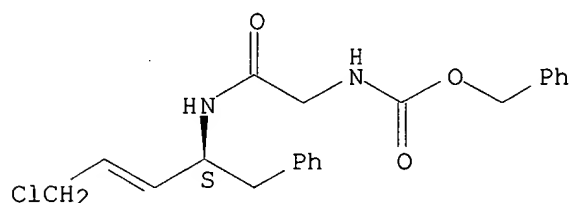
MF C21 H23 Cl N2 O3

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 21 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 173866-67-6 REGISTRY

CN Carbamic acid, [2-[[4-bromo-1-(phenylmethyl)-2-butenyl]amino]-2-oxoethyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

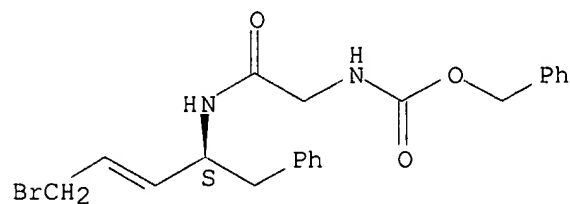
MF C21 H23 Br N2 O3

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

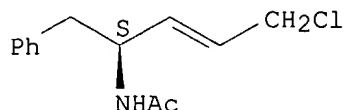
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1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 22 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 173866-64-3 REGISTRY
 CN Acetamide, N-[4-chloro-1-(phenylmethyl)-2-butenyl]-, (S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C13 H16 Cl N O
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.
 Double bond geometry unknown.



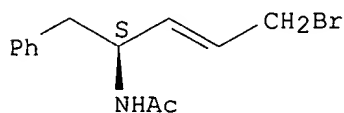
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1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

L59 ANSWER 23 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 173866-63-2 REGISTRY
 CN Acetamide, N-[4-bromo-1-(phenylmethyl)-2-butenyl]-, (S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C13 H16 Br N O
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.
 Double bond geometry unknown.



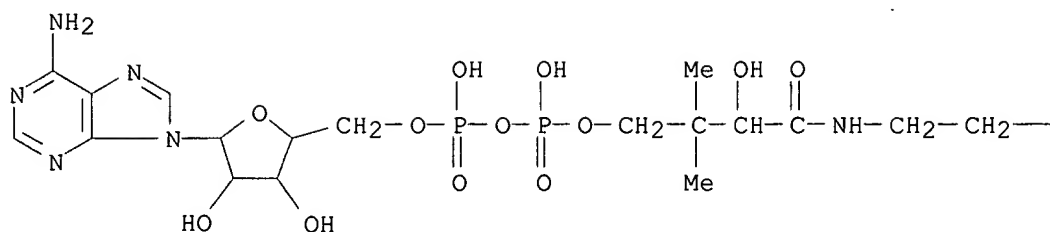
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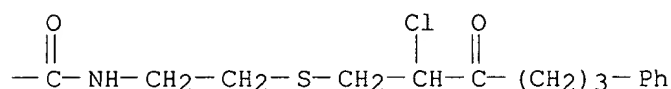
REFERENCE 1: 124:169116

L59 ANSWER 24 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 128409-68-7 REGISTRY
 CN Coenzyme A, S-(2-chloro-3-oxo-6-phenylhexyl)- (9CI) (CA INDEX NAME)
 MF C33 H48 Cl N7 O14 P2 S
 SR CA
 LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

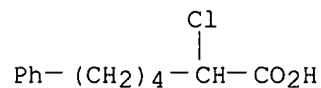


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:56233

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L59 ANSWER 25 OF 47  REGISTRY  COPYRIGHT 2002 ACS
RN 128409-67-6  REGISTRY
CN Benzenehexanoic acid, .alpha.-chloro- (9CI)  (CA INDEX NAME)
FS 3D CONCORD
DR 128409-71-2
MF C12 H15 Cl O2
SR CA
LC STN Files:  CA, CAPLUS, MEDLINE
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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

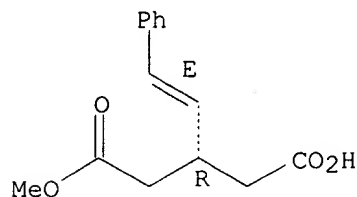
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:56233

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L59  ANSWER 26 OF 47  REGISTRY  COPYRIGHT 2002 ACS
RN   117214-00-3  REGISTRY
CN   Pentanedioic acid, 3-(2-phenylethenyl)-, monomethyl ester, [R-(E)]- (9CI)
      (CA INDEX NAME)
FS   STEREOSEARCH
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MF C14 H16 O4
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Absolute stereochemistry.
 Double bond geometry as shown.



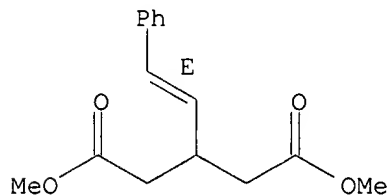
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:186743

L59 ANSWER 27 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 117213-93-1 REGISTRY
 CN Pentanedioic acid, 3-(2-phenylethenyl)-, dimethyl ester, (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C15 H18 O4
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

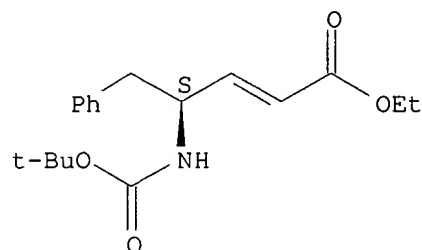
REFERENCE 1: 110:74799

REFERENCE 2: 109:186743

L59 ANSWER 28 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 116246-06-1 REGISTRY
 CN 2-Pentenoic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-5-phenyl-, ethyl

ester, (S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C18 H25 N O4
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
 (*File contains numerically searchable property data)

Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:169116

REFERENCE 2: 113:153049

REFERENCE 3: 109:129688

L59 ANSWER 29 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN **99858-37-4** REGISTRY
 CN Benzene, (5-iodopentyl)- (6CI, 9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN (5-Iodopentyl)benzene
 CN 1-Iodo-5-phenylpentane
 CN 5-Phenyl-1-iodopentane
 FS 3D CONCORD
 MF C11 H15 I
 SR CAOLD
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)

I- (CH₂)₅- Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1967 TO DATE)
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 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 134:207397

REFERENCE 2: 133:222752
 REFERENCE 3: 130:267212
 REFERENCE 4: 130:52236
 REFERENCE 5: 130:3689
 REFERENCE 6: 124:8857
 REFERENCE 7: 123:143878
 REFERENCE 8: 122:313813
 REFERENCE 9: 113:77634

L59 ANSWER 30 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN **93383-65-4** REGISTRY

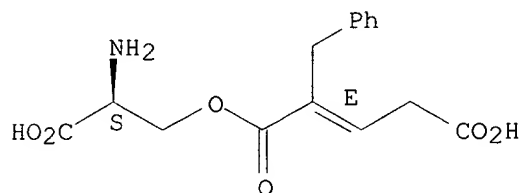
CN L-Serine, 5-hydrogen 2-(phenylmethyl)-2-pentenedioate (ester), (E)- (9CI)
 (CA INDEX NAME)

FS STEREOSEARCH

MF C15 H17 N O6

LC STN Files: CA, CAPLUS

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 102:2495

L59 ANSWER 31 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN **89094-76-8** REGISTRY

CN 18,19-Dinorpregn-4-en-20-yn-3-one, 13-ethyl-17-[(1-oxo-5-phenyl-2-penten-4-ynyl)oxy]-, [17.alpha.,17(E)]- (9CI) (CA INDEX NAME)

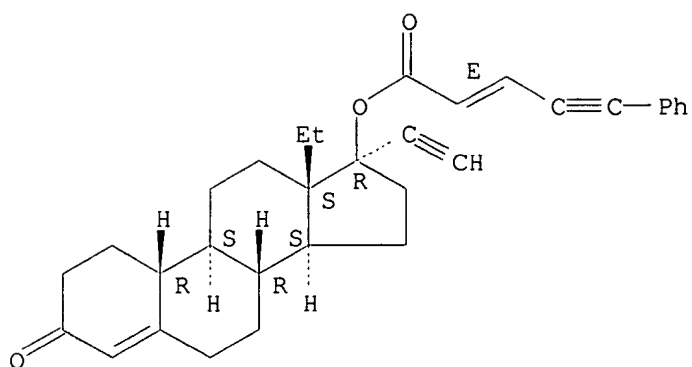
FS STEREOSEARCH

MF C32 H34 O3

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 102:154799

REFERENCE 2: 100:115151

REFERENCE 3: 100:115135

L59 ANSWER 32 OF 47 REGISTRY COPYRIGHT 2002 ACS

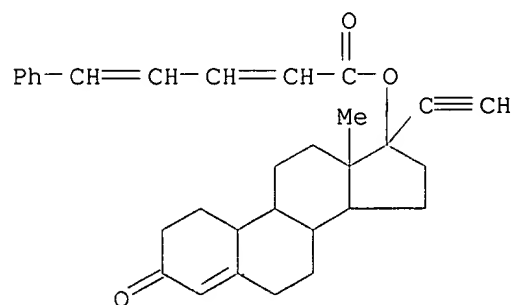
RN **89094-62-2** REGISTRY

CN 19-Norpregn-4-en-20-yn-3-one, 17-[(1-oxo-5-phenyl-2,4-pentadienyl)oxy]-,
[17.alpha.,17(2E,4E)]- (9CI) (CA INDEX NAME)

MF C31 H34 O3

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

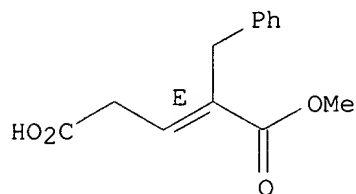
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 100:115151

REFERENCE 2: 100:115135

L59 ANSWER 33 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 85533-91-1 REGISTRY
 CN 2-Pentenedioic acid, 2-(phenylmethyl)-, 1-methyl ester, (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C13 H14 O4
 LC STN Files: CA, CAPLUS

Double bond geometry as shown.



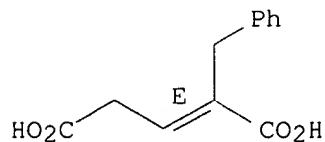
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:18590

L59 ANSWER 34 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 85533-88-6 REGISTRY
 CN 2-Pentenedioic acid, 2-(phenylmethyl)-, (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C12 H12 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

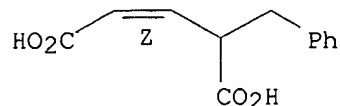
REFERENCE 1: 102:2495

REFERENCE 2: 99:18590

L59 ANSWER 35 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 85533-85-3 REGISTRY
 CN 2-Pentenedioic acid, 4-(phenylmethyl)-, (Z)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH

MF C12 H12 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Double bond geometry as shown.



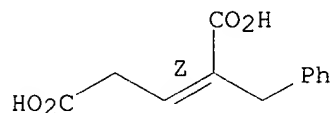
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:18590

L59 ANSWER 36 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN **85533-84-2** REGISTRY
 CN 2-Pentenedioic acid, 2-(phenylmethyl)-, (Z)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C12 H12 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Double bond geometry as shown.



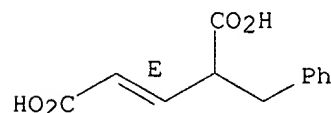
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:18590

L59 ANSWER 37 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN **85533-83-1** REGISTRY
 CN 2-Pentenedioic acid, 4-(phenylmethyl)-, (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C12 H12 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Double bond geometry as shown.



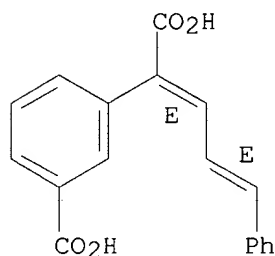
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:18590

L59 ANSWER 38 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN **81995-43-9** REGISTRY
CN Benzeneacetic acid, 3-carboxy-.alpha.-(3-phenyl-2-propenylidene)-, (E,E)-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H14 O4
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 97:91946

L59 ANSWER 39 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN **52121-98-9** REGISTRY
CN Benzene, (6-iodohexyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Iodo-6-phenylhexane
CN 6-Phenyl-1-iodohexane
CN 6-Phenylhexyl iodide
FS 3D CONCORD
MF C12 H17 I
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB,
TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

I-(CH₂)₆-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1967 TO DATE)

14 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:295024
 REFERENCE 2: 130:267212
 REFERENCE 3: 130:52236
 REFERENCE 4: 130:3689
 REFERENCE 5: 126:277342
 REFERENCE 6: 125:167772
 REFERENCE 7: 125:58199
 REFERENCE 8: 123:143878
 REFERENCE 9: 122:239193
 REFERENCE 10: 113:77634

L59 ANSWER 40 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN **37566-49-7** REGISTRY

CN 4-Hexyn-3-one, 6-bromo-1-phenyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

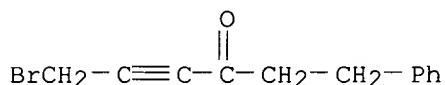
CN 6-Bromo-1-phenylhex-4-yn-3-one

FS 3D CONCORD

MF C12 H11 Br O

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:71959

L59 ANSWER 41 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN **34807-41-5** REGISTRY

CN 2,4-Pentadienoic acid, 5-phenyl-, (2S,3aR,3bS,3cS,4aR,5S,5aS,8aR,8bR,9R,10R,10aS)-3a,3b,3c,4a,5,5a,8a,9,10,10a-decahydro-5,5a-dihydroxy-4a-(hydroxymethyl)-7,9-dimethyl-10a-(1-methylethenyl)-6-oxo-2-phenyl-6H-2,8b-epoxyoxireno[6,7]azuleno[5,4-e]-1,3-benzodioxol-10-yl ester, (2E,4E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Daphnetoxin, 12-[(1-oxo-5-phenyl-2,4-pentadienyl)oxy]-, [12.beta.(2E,4E)]-

OTHER NAMES:

CN 2,4-Pentadienoic acid, 5-phenyl-, 3a,3b,3c,4a,5,5a,8a,9,10,10a-decahydro-5,5a-dihydroxy-4a-(hydroxymethyl)-7,9-dimethyl-10a-(1-methylethenyl)-6-oxo-2-phenyl-6H-2,8b-epoxyoxireno[6,7]azuleno[5,4-e]-1,3-benzodioxol-10-yl

ester, [2S-[2.alpha.,3a.beta.,3b.beta.,3c.beta.,4a.beta.,5.beta.,5a.beta.,
8a.alpha.,8b.alpha.,9.alpha.,10.beta.(2E,4E),10a.beta.]]-

CN Meserein

CN Mezerein

CN Mezereine

CN NSC 239072

FS STEREOSEARCH

DR 30220-44-1, 32207-09-3

MF C38 H38 O10

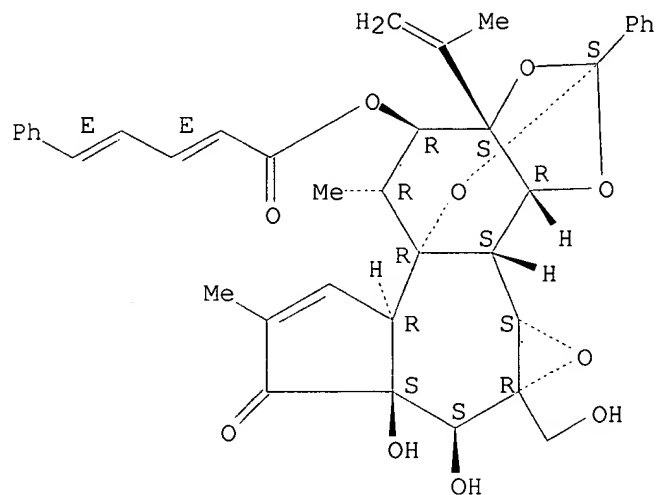
CI COM

LC STN Files: ADISINSIGHT, AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS,
BIOTECHNO, CA, CANCERLIT, CAPLUS, CHEMCATS, CIN, CSCHEM, DDFU, DRUGU,
EMBASE, MEDLINE, NAPRALERT, NIOSHTIC, PROMT, RTECS*, TOXCENTER,
USPATFULL

(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

432 REFERENCES IN FILE CA (1967 TO DATE)

433 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:288676

REFERENCE 2: 136:148710

REFERENCE 3: 136:31428

REFERENCE 4: 136:15800

REFERENCE 5: 135:284382

REFERENCE 6: 134:348688

REFERENCE 7: 134:261200

REFERENCE 8: 134:141737

REFERENCE 9: 134:1524

REFERENCE 10: 133:358827

L59 ANSWER 42 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 28010-13-1 REGISTRY

CN 2,4-Pentadienoic acid, 5-phenyl-, (Z,E)- (8CI, 9CI) (CA INDEX NAME)

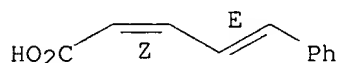
FS STEREOSEARCH

MF C11 H10 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX

(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

14 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:56016

REFERENCE 2: 121:157229

REFERENCE 3: 116:151455

REFERENCE 4: 116:2232

REFERENCE 5: 110:121165

REFERENCE 6: 107:77283

REFERENCE 7: 96:104596

REFERENCE 8: 94:151746

REFERENCE 9: 93:203839

REFERENCE 10: 91:210563

L59 ANSWER 43 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 28010-12-0 REGISTRY

CN 2,4-Pentadienoic acid, 5-phenyl-, (2E,4E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2,4-Pentadienoic acid, 5-phenyl-, (E,E)- (8CI)

OTHER NAMES:

CN (2E,4E)-5-Phenyl-2,4-pentadienoic acid

CN (2E,4E)-Cinnamylideneacetic acid

CN (E,E)-5-Phenyl-2,4-pentadienoic acid

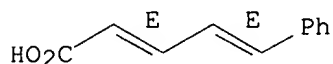
CN .alpha.-trans-.gamma.-trans-.beta.-Styrylacrylic acid

CN 5-Phenyl-2E,4E-pentadienoic acid

CN 5-Phenyl-trans-2,trans-4-pentadienoic acid

FS STEREOSEARCH
 MF C11 H10 O2
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX, TOXCENTER,
 USPATFULL
 (*File contains numerically searchable property data)

Double bond geometry as shown.

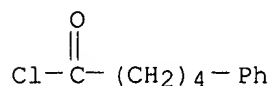


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

50 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 50 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:294651
 REFERENCE 2: 136:279218
 REFERENCE 3: 135:366118
 REFERENCE 4: 135:195169
 REFERENCE 5: 135:192530
 REFERENCE 6: 134:280547
 REFERENCE 7: 132:307866
 REFERENCE 8: 131:322807
 REFERENCE 9: 130:95351
 REFERENCE 10: 130:52013

L59 ANSWER 44 OF 47 REGISTRY COPYRIGHT 2002 ACS
 RN 20371-41-9 REGISTRY
 CN Benzenepentanoyl chloride (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Valeryl chloride, 5-phenyl- (8CI)
 OTHER NAMES:
 CN 5-Phenylpentanoyl chloride
 CN 5-Phenylvaleryl chloride
 FS 3D CONCORD
 MF C11 H13 Cl O
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB,
 TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)

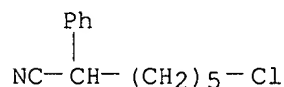


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

65 REFERENCES IN FILE CA (1967 TO DATE)
65 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:282685
REFERENCE 2: 135:253261
REFERENCE 3: 135:210837
REFERENCE 4: 135:92538
REFERENCE 5: 133:321879
REFERENCE 6: 132:264741
REFERENCE 7: 132:208142
REFERENCE 8: 132:78577
REFERENCE 9: 131:351322
REFERENCE 10: 131:214285

L59 ANSWER 45 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN **14377-66-3** REGISTRY
CN Benzeneacetonitrile, .alpha.-(5-chloropentyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Heptanenitrile, 7-chloro-2-phenyl- (8CI)
FS 3D CONCORD
MF C13 H16 Cl N
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)



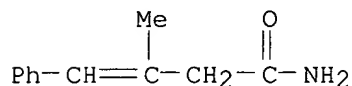
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:74591
REFERENCE 2: 120:244331
REFERENCE 3: 66:94792

L59 ANSWER 46 OF 47 REGISTRY COPYRIGHT 2002 ACS
RN **7236-47-7** REGISTRY
CN 3-Butenamide, 3-methyl-4-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:

CN .beta.-Benzalbutyramide
 CN 3-Methyl-4-phenyl-3-butenamide
 CN 3-Methyl-4-phenyl-3-butenic acid amide
 CN Kata-Lipid
 CN Lipidemol
 CN Lipobeta
 FS 3D CONCORD
 MF C11 H13 N O
 LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CHEMCATS, CHEMLIST,
 CSCHEM, HODOC*, IPA, MEDLINE, MRCK*, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**
 (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

17 REFERENCES IN FILE CA (1967 TO DATE)
 17 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:273206
 REFERENCE 2: 134:530
 REFERENCE 3: 132:73218
 REFERENCE 4: 88:16047
 REFERENCE 5: 81:169330
 REFERENCE 6: 76:43361
 REFERENCE 7: 75:86118
 REFERENCE 8: 72:131022
 REFERENCE 9: 72:120015
 REFERENCE 10: 72:88824

L59 ANSWER 47 OF 47 REGISTRY COPYRIGHT 2002 ACS

RN 1516-24-1 REGISTRY

CN 2,4-Pentadienoic acid, 5-phenyl-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA
 INDEX NAME)

OTHER NAMES:

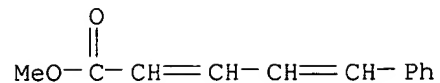
CN Methyl 4-phenylbutadienecarboxylate

CN Methyl 5-phenyl-2,4-pentadienoate

FS 3D CONCORD

MF C12 H12 O2

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMINFORMRX,
 HODOC*, USPATFULL
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

20 REFERENCES IN FILE CA (1967 TO DATE)
20 REFERENCES IN FILE CAPLUS (1967 TO DATE)
7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 130:81047
REFERENCE 2: 127:304705
REFERENCE 3: 125:85964
REFERENCE 4: 125:58265
REFERENCE 5: 124:202303
REFERENCE 6: 119:8882
REFERENCE 7: 113:114384
REFERENCE 8: 110:8600
REFERENCE 9: 108:21792
REFERENCE 10: 106:84485